## GEORGIA INSTITUTE OF TECHNOLOGY Engineering Experiment Station Atlanta, Georgia

FINAL REPORT

PROJECT A-831

STUDY OF THE METHODS FOR THE NUMERICAL SOLUTION OF ORDINARY DIFFERENTIAL EQUATIONS

Ву

L.J. GALLAHER, G.E. DUNCAN, O.B. FRANCIS, JR., J.M. GWYNN, JR., H.G. HALE, JR., and I.E. PERLIN

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#### ABSTRACT

This report outlines the work accomplished and results achieved in the preparation of a computer procedure for the integration of ordinary differential equations. The following characteristics of the programs are specified:

- a) The procedure for integration must achieve the accuracy specified by the user.
- b) The procedure must be problem independent and applicable to the integration of any degree or number of coupled differential equations.
- c) The step size, order and method of integration are to be chosen so as to minimize computation time while meeting the accuracy requirements.
- d) The procedure is to have built-in learning so that previous experience can be used from one call to the next to decide on the method and order to be used. The procedure is to be self-modifying.

The following methods were used in the development of the procedure.

- a) Adams-Bashforth-Moulton
- b) Stetter-Gragg-Butcher
- c) Cowell's method of constant Nth order difference
- d) Runge-Kutta-Shanks.

Four different orders were used for each of the above methods.

Information is provided on an executive procedure developed to act in an administrative and bookkeeping capacity for the basic integration routines indicated above, plus a start and restart routine, which contains a separate Runge-Kutta-Shanks routine. This executive procedure works very satisfactorily.

Three types of problems were used to exercise this procedure. These three types are the Arenstorf orbits of the restricted three body problem, the system of linear differential equations associated with Fourier transforms, and the

system of linear equations obtained from the partial differential equation for the vibrating string.

The results of running with a variety of problems and accuracies are that no particular method seems very superior to any other. All methods performed well.

The results justify the conclusion that the program developed would be very useful as a general library program for integrating systems of differential equations.

Several suggestions for further study are outlined in Chapter IV.

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#### I. INTRODUCTION

In previous work done under this contract, an effort was made to determine which of the many methods and orders available for integrating ordinary differential equations was best. While it was possible to show that, under certain circumstances, some methods and orders outperformed others, no one method was clearly superior under all circumstances.

In the present contract, the goal was set of writing a computer program for the integration of systems of ordinary differential equations (initial value problems), characterized by the following specifications:

- a) The integration must meet a (user's) specified accuracy.
- b) The procedure will be problem independent and applicable to the integration of any degree or number of coupled differential equations.
- c) The step size, order, and method of integration are to be chosen by the procedure so as to be optimum; that is, to minimize the computation time while meeting the accuracy requirements.
- d) The procedure will have built-in learning so that it can use its experience from one call to the next to decide on the method and order to be used. The procedure will be self-modifying.

The methods used are as follows:

- (1) The Adams-Bashforth-Moulton method,
- (2) The Stetter-Gragg-Butcher method,
- (3) Cowell's method of constant Nth order differences,
- (4) The Runge-Kutta-Shanks method.

With each of these methods, four different orders are used. A history file is kept showing the past performance scores of each method and order and is used to select which methods and orders are to be employed.

The program works in the following way. When a call is made in the procedure to integrate from point a to the point b, this interval is divided into eighths. The first eighth of the interval is integrated by one method for each of two different orders, and the times taken by each recorded. The second eighth is integrated by another method, also for two different orders, and the times recorded. The winners then compete against each other over the next fourth of the interval. That is, the fastest order of the first method and the faster order of the second method are both used to integrate the second fourth of the interval, and the times taken by each recorded. The faster method of these two is then presumably the best (fastest) of the four tried, and it is used (alone) to integrate over the last half of the interval. All of the times measured above are then logged in a cumulative history file and the winners and losers noted.

This history file then is used as the basis for selecting which methods and orders are chosen each time.

The first of the two methods is chosen at random (using a random number generator) from among the four available. The second method is chosen to be the method showing the best history of success among the three remaining methods, with the cumulative history file being used to determine the degree of success. Then within each method the same kind of selection process with respect to orders is used. That is, the first order is chosen at random, and the second order is chosen on the basis of which of the remaining three has been the most successful (fastest running) order of that method. Thus it is seen that the past performance of the different methods and orders influences the choice of which are allowed to compete, such that the more successful have a higher probability of being selected.

In using time as the sole estimate of performance efficiency, it is assumed that all orders and methods have satisfactorily met the accuracy requirements. The accuracy requirements of each method are met by controlling step size and making error estimates at each step. The method of error estimate is different for the different methods. In the Runge-Kutta single step method, the error is estimated by taking two half steps and then a whole step. In the Adams and Butcher methods the difference between predictor and corrector is used. In the Cowell method a mid-range formula is used. (Only in the Adams and the Runge-Kutta cases is there good theoretical justification for using these methods to calculate the actual error -- the error estimates in the Butcher and Cowell methods are essentially empirical.)

One further feature introduced into the learning process is the gradual "forgetting" of events in the more distant past. This causes the events in the distant past to have less influence than those more recent in determining the score or performance figure of an order and method.

Three types of problems were used to exercise the integration procedure:

First, the Arenstorf type orbits of the restricted three body

problem (four equations).

Second, the system of linear differential equations associated with the Fourier transforms (20 to 40 equations).

Third, the system of linear differential equations obtained from a discretization of the partial differential equation for the vibrating string (50 to 100 equations).

The first of these is characterized by the necessity of frequent step size change. The other two have no need for step size change once the correct step is found.

The preliminary results of running with a variety of problems and accuracies is that no particular method seems to be exceptionally superior to any other. It did appear that, for the accuracy range used, certain orders of some methods were inappropriate. Also, for a given method one particular order usually dominated, but which one dominated depended on the accuracy being asked and to some extent the problem. In any event the program adapted quite rapidly to the characteristics of a particular problem and accuracy.

All methods performed well and, for different problems, different methods showed up more successfully. For example, the Runge-Kutta method was most successful when frequent step size changes were required, but the multistep methods performed better when long runs of uniform step size were appropriate.

The results justify the conclusion that the present program would be suitable and effective as a general library program for integrating systems of differential equations.

#### II. INTEGRATION METHODS

### A. The Method of Adams, Bashforth and Moulton

#### 1. Description of the Method

The method investigated consists of the combination of two different versions of the method of Adams into a predictor-corrector system [5]. The use of this system to obtain numerical solutions to a set of simultaneous differential equations with given initial conditions is independent both of the number of equations in the set to be solved and of the orders of the individual equations in the set; provided, however, that each equation of order m is expressed as a set of m coupled first order equations.

In general then, one deals with the system of equations

$$\vec{y}'(x) \equiv \frac{d}{dx} \vec{y}(x) = \vec{f}(x, \vec{y}(x)), \qquad (1-1)$$

where  $\vec{y}$ ,  $\vec{y}$ , and  $\vec{f}$  are vectors, each having a number of components, N, equal to  $\sum_{i=1}^k m_i$ , where k is the number of equations in the set to be solved, and the  $m_i$  are their individual orders.

This vector differential equation is equivalent to the integral equation

$$\vec{y}(x+h) = \vec{y}(x) + \int_{x}^{x+h} \vec{f}(t, \vec{y}(t)) dt.$$
 (1-2)

At the point  $x = x_q \equiv x_{q-1} + h$ , this integral is approximated first by

$$\vec{y}_{q}^{(0)} = \vec{y}_{q-1} + h \sum_{\mu=0}^{q-1} \beta_{q-1, q-1-\mu} \vec{f}_{\mu}$$
 (1-3a)

and then repeatedly by

$$\vec{y}_{q}^{(\nu+1)} = h\beta_{q,o}^{*}\vec{f}(x_{q},\vec{y}^{(\nu)}(x_{q})) + h\sum_{\mu=0}^{q-1}\beta_{q,q-\mu}^{*}\vec{f}_{\mu}$$

$$\equiv h\beta_{q,o}^{*}\vec{f}_{q}^{(\nu)} + \vec{c}, \nu=0,1,2, \dots (1-3b)$$

which converges toward  $\vec{y}_q \equiv \vec{y}(x_q)$  as  $\nu$  increases. Formula (1-3a) is called the Adams-Bashforth predictor equation, and formula (1-3b) is the Adams-Moulton corrector.

The coefficients  $\beta_{q\rho}$  and  $\beta_{q\rho}^*$  are derived by the equivalent of integrating Lagrangian polynomials fitted to  $\vec{f}$ , but are independent of both  $\vec{f}$  and h. The polynomial for the predictor is of degree q-l passing through the q points  $\vec{f}_0$ ,  $\vec{f}_1$ , . . .,  $\vec{f}_{q-1}$ , while that for the corrector is of degree q passing through the q + l points  $\vec{f}_0$ ,  $\vec{f}_1$ , . . .,  $\vec{f}_q$ .

An explicit formula for the  $\beta_{\alpha\rho}$  is

$$\beta_{q\rho} = (-1)^{\rho} \left\{ \binom{\rho}{\rho} \gamma_{\rho} + \binom{\rho+1}{\rho} \gamma_{\rho+1} + \dots + \binom{q}{\rho} \gamma_{q} \right\}, \begin{array}{l} q = 0, 1, 2, \dots \\ \rho = 0, 1, \dots, q \end{array}$$

where the  $\binom{\rho+i}{\rho}$  represent binomial coefficients and the  $\gamma_\rho$  are found by the recursion relation

$$\gamma_{\rho} + \frac{1}{2} \gamma_{\rho-1} + \dots + \frac{1}{\rho+1} \gamma_{o} = 1, \quad \rho = 0, 1, 2, \dots,$$

and an explicit formula for the  $\beta_{q\rho}^{*}$  is

$$\beta_{q0}^{*} = (-1)^{\rho} \left\{ \binom{\rho}{\rho} \gamma_{0}^{*} + \binom{\rho+1}{\rho} \gamma_{\rho+1}^{*} + \dots + \binom{q}{\rho} \gamma_{q}^{*} \right\}, \quad q = 0, 1, 2, \dots, q$$

where 
$$\gamma_0^* = 1$$
 and  $\gamma_\rho^* = \gamma_\rho - \gamma_{\rho-1}$ ,  $\rho = 1,2,3, \dots$ 

Bounds on the errors for the two approximations are the maximums within the interval  $[x_0, x_q]$  of

and of

and M, the order of the predictor-corrector system, is assumed to approximate that of the corrector, which is q + 1.

## 2. The Computer Procedure

The procedure ADAMS itself is written to be included in programs written in single precision for the Burroughs B-5500 computer. The language is Algol 60 augmented by additional features available in the Algol compiler for the B-5500. There are no unusual hardware requirements, because all input and output to the procedure is under control of the including program through the formal parameter list. All variables not in the formal parameter list are local to the procedure, and no files are used by the procedure.

# 2.1 Parameters and Variables

The following lists of formal parameters and local variables will be useful in describing the operation of procedure ADAMS. In the remainder of this discussion the interchange of upper and lower case letters, necessitated

by approximating the notation [5] within the limited character set available to a computer, is straight-forward and will be done freely without further comment.

## Formal Parameters

Identifier	Type	Usage or Meaning
N	Integer	The number of components in the vectors $\vec{y}$ , $\vec{E}A$ , and $\vec{E}R$ .
XI	Real	Initial value of the independent variable.
XF	Real	Final value of the independent variable.
Y	Real Array	Current dependent variable vector. Contains initial values at entry and final values at exit.
F	Procedure	Calculates the vector $\vec{f}(x,\vec{y}(x))$ .
P	Real	Power of Cl used in error control.
ବ	Integer	Number of back $\vec{f}$ points used in the approximating polynomials. One less than M, the order of the method.
DX	Real	Upper bound on the initial step size.
EA	Real Array	Absolute error bound vector.
ER	Real Array	Relative error bound vector.
ADAMSCOEFF	. Real Array	Contains the $\beta_{q\rho}$ , the $\beta_{q\rho}^*$ , and $\begin{vmatrix} 1 - \gamma_{q+1}/\gamma_{q+1}^* \end{vmatrix}$ .
RKSFNS	Integer	Function evaluations per step for procedures START and SHANKS.
RKSORDER	Integer	Order of R.K.S. method to be used by START and SHANKS.
RKSCOEFF	Real Array	Coefficients for START and SHANKS. See the desciptions of START and SHANKS elsewhere in this report for details.
START	Integer Procedure	Gives the necessary points for starting and restarting. Name contains the factor by which Cl is multiplied to coordinate step size between START and ADAMS.
SHANKS	Procedure	Used to complete fractional steps at the ends of intervals.

The procedures START, SHANKS, and F, as well as the coefficient arrays ADAMSCOEFF and RESCOEFF, are not a part of the procedure ADAMS and must be included separately in all programs using ADAMS (see 2.2 and 2.3).

# Local Variables

Identifier	Type	Usage or Meaning
X	Real	$\mathbf{x}_{\mathbf{q}}$ , current value of the independent variable.
INTERVAL	Real	XF - XI, the interval of integration.
Cl	Integer	Two to an integral power. Determines H.
Н	Real	INTERVAL / Cl, the current step size.
C2	Real	Number of steps of size H remaining from X to XF.
GR	Real	$1 - \gamma_{q+1}/\gamma_{q+1}^*$ , used with CHANGE and ERROR.
CHANGE	Real	Controls the number of iterations of the corrector equation.
ERROR	Real	Controls the error and running time through the step size.
FP	Real Array	Predicted $\vec{y}_q'$ vector, $\vec{f}_q^{(p)}$ , the $\vec{f}_q^{(v)}$ of (1-3b).
FC	Real Array	Corrected $\vec{y}'_q$ vector, $\vec{f}^{(c)}$ , $\vec{f}_q^{(v+1)}$ in (1-3b).
FH	Real Array	$\vec{f}$ history vector. Contains 2q-1 back points for each of the N components of $\vec{f}$ .
ΥP	Real Array	Predicted $\vec{y}_q$ vector, $\vec{y}^{(p)}$ , the $\vec{y}_q^{(o)}$ of (1-3a).
YC	Real Array	Corrected $\vec{y}_q$ vector, $\vec{y}^{(c)}$ , the $\vec{y}_q^{(v+1)}$ of (1-3b).
ΥB	Real Array	Back $\vec{y}$ vector, $\vec{y}^{(b)}$ , needed for restarting after halving.
VD.	Real Array	Alternate YB.

All local arrays are dynamic with respect to N and Q and, to avoid moving large numbers of components, reversals in meaning are made on successive

steps or iterations between FP and FC, between YP and YC, and between YB and YD. The FH vector array is indexed cyclically for the same reason. For further details consult the flow diagram and the listing of procedure ADAMS following this discussion.

### 2.2 The F Procedure

A procedure for calculating the vector  $\vec{y}' = \vec{f}(x, \vec{y}(x))$  must be included global to a call for procedure ADAMS for each set of differential equations to be solved by a program using ADAMS. This procedure is called by ADAMS as the formal parameter F and must itself have the following formal parameter list:

<u>Identifier</u>	Type	Usage or Meaning
N	Integer	Number of components in the vectors YV and FV.
X	Real	Current value of the independent variable.
ΥV	Real Array	Current dependent variable vector (input).
FV	Real Array	F value vector (output).

N and X may be called by value. The arrays YV and FV are onedimensional starting at zero and must be called by name.

### 2.3 Orders Available

The procedure ADAMS is written to be completely general with regard to order, and any order may be used if the necessary coefficients are placed in the ADAMSCOEFF array. For a given order M=q+1, there are 2q+2=2M coefficients which should appear in the array beginning at position zero in the following order:

$$\beta_{q-1,q-1}, \ \beta_{q-1,q-2}, \ \dots, \ \beta_{q-1,o}, \ \beta_{q,q}^*, \beta_{q,q-1}^*, \ \dots, \beta_{q,o}^*, \left| 1-\gamma_{q+1}/\gamma_{q+1}^* \right|.$$

# 2.4 Starting an Integration

Since the Adams method is a multistep method it cannot start itself but must rely on a starting procedure that will supply at least q-1  $\vec{f}$  points which, together with a given initial  $\vec{f}$  point and a current  $\vec{y}$  point, comprise a history upon which it can build. The starting procedure used here is the Runge-Kutta-Shanks procedure START, described elsewhere in this report. The number of function evaluations per step and the order of Runge-Kutta-Shanks method used by START may be varied at will by the user through the formal parameters of ADAMS. This will achieve optimum compatibility with the order of Adams method being used for each given set of differential equations being solved.

Initial step size is determined by the formal parameter DX. The initial trial start will be made with a step H = INTERVAL / Cl, where Cl is set to the smallest integer power of two such that  $|H| \leq |DX|$  and  $|H| \leq |INTERVAL|/Q$ . This causes the prodecure ADAMS to take at least one step after starting regardless of the magnitude of DX. If the procedure START cannot meet the error requirements at the initial H, it doubles Cl repeatedly until these requirements can be met.

### 2.5 Error Estimates and Step Size Control

To minimize running time without introducing errors intolerably large, the error in each component of the final  $\vec{Y}$  vector is controlled through the use of the formal parameters  $\vec{EA}$  and  $\vec{ER}$ .  $\vec{EA}$  specifies the maximum allowable absolute magnitude of the error in each component of  $\vec{Y}$ , and  $\vec{ER}$  specifies the maximum allowable relative magnitude. These two error control vectors are used in conjunction with the quantity  $GR = \left|1-\gamma_q\right|\gamma_{q+1}^*$ , which is derived from the bounds (1-4), and a parameter P, chosen from the interval  $\left[\frac{1}{2},1\right]$  by

empirical determination of the randomness of the round-off error in a particular set of differential equations. (P =  $\frac{1}{2}$  corresponds to totally random error and P = 1 corresponds to totally additive error.) In practice  $\gamma_{q+1}$  has been used in GR instead of  $\gamma_q$  to be conservative, because the quantity being controlled is only an estimate of the true error.

The estimated error vector  $\overrightarrow{ERROR}$  is defined to be  $|\overrightarrow{y} - \overrightarrow{y}|$ , where  $\overrightarrow{y}^{(p)}$  is the  $\overrightarrow{y}_q^{(o)}$  of (1-3a) and  $\overrightarrow{y}^{(c)}$  is  $\overrightarrow{y}_q^{(v_f+1)}$  in (1-3b), with  $v_f$  being the first v for which every component of

$$\overrightarrow{\text{CHANGE}} \equiv |\overrightarrow{f}_{q}^{(\nu+1)} - \overrightarrow{f}_{q}^{(\nu)}| = |(\overrightarrow{y}_{q}^{(\nu+1)} - \overrightarrow{y}_{q}^{(\nu)}) / h\beta_{q,0}^{*}|$$

is less than the corresponding component of either

$$\left| \frac{\vec{EA} \cdot \vec{GR}}{\vec{Cl}^P \cdot 2^{Q+5} \cdot \vec{h\beta}_{q,0}^*} \right| \quad \text{or} \quad \left| \frac{\vec{ER} \cdot \vec{GR}}{\vec{Cl}^P \cdot 2^{Q+5} \cdot \vec{h\beta}_{q,0}^*} \cdot \vec{f}_q^{(v+1)} \right| .$$

If any component of ERROR is larger than the corresponding components of both

and

$$\left| \frac{\vec{ER} \cdot GR}{Cl^{P}} \cdot \vec{y}^{(c)} \right|,$$

then  $\vec{y}$  is replaced by  $\vec{y}^{(b)}$ , the step size is halved, and q-l new  $\vec{f}$  points and a new current  $\vec{y}$  are obtained from the procedure START. If it is not necessary to halve the step size, then  $\vec{y}^{(c)}$  becomes the new  $\vec{y}$ . If every component of  $\vec{f}$  is smaller for three consecutive steps than the corresponding components of both

$$\begin{vmatrix} \vec{EA} \cdot GR \\ Cl^{P} \cdot 2^{Q+5} \end{vmatrix} \text{ and } \begin{vmatrix} \vec{ER} \cdot GR \\ Cl^{P} \cdot 2^{Q+5} \end{vmatrix} \cdot \vec{y}^{(c)} \end{vmatrix},$$

then if there are at least 2q-1 back points in the  $\overrightarrow{FH}$  array and there are at least two more steps of the current size necessary to reach XF, the step size is doubled before the next trial step. If it is not necessary either to halve or to double the step size, X is increased by H and a new trial step is made.

### 2.6 Finishing an Integration

The procedure ADAMS continues as described until XF is reached unless repeated halvings and doublings of the step size bring the independent variable to within a fraction of a single step of XF. When this occurs, the fractional step is completed by the Runge-Kutta-Shanks procedure SHANKS, described elsewhere in this report. The order of Runge-Kutta-Shanks method and the number of function evaluations per step used here will be the same for a given integration as those used by the procedure START.

### 3. Flow Diagram and Program Listing

Figure 1 is the flow diagram for the method of Adams, Bashforth and Moulton. The program listing follows at the end of this section.

#### 4. Results and Conclusions

For experimental and diagnostic reasons, the procedure ADAMS was originally checked out with separate arrays for the dependent variable vectors  $\overrightarrow{YI}$  (initial values),  $\overrightarrow{YB}$  (back values), and  $\overrightarrow{YF}$  (final values), all of which are now made equivalent to  $\overrightarrow{Y}$  in the DEFINE statement. These arrays may be removed from the define statement and declared to be local arrays, global arrays, or formal parameters if any reason for doing so should arise. If this is done  $\overrightarrow{Y}$  should be removed from the formal parameter list.

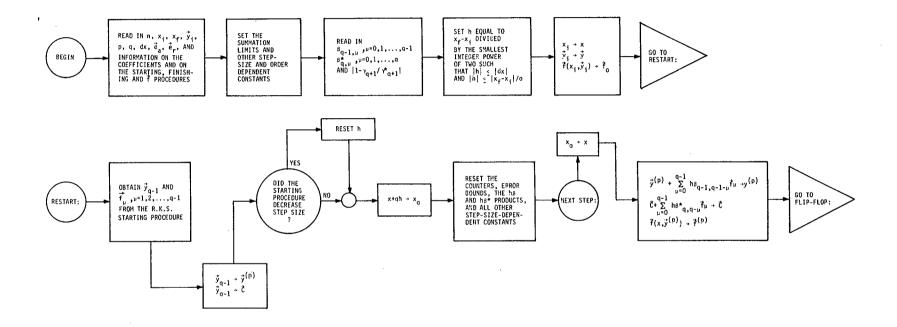


Figure 1. Flow Diagram for the Adams Method.

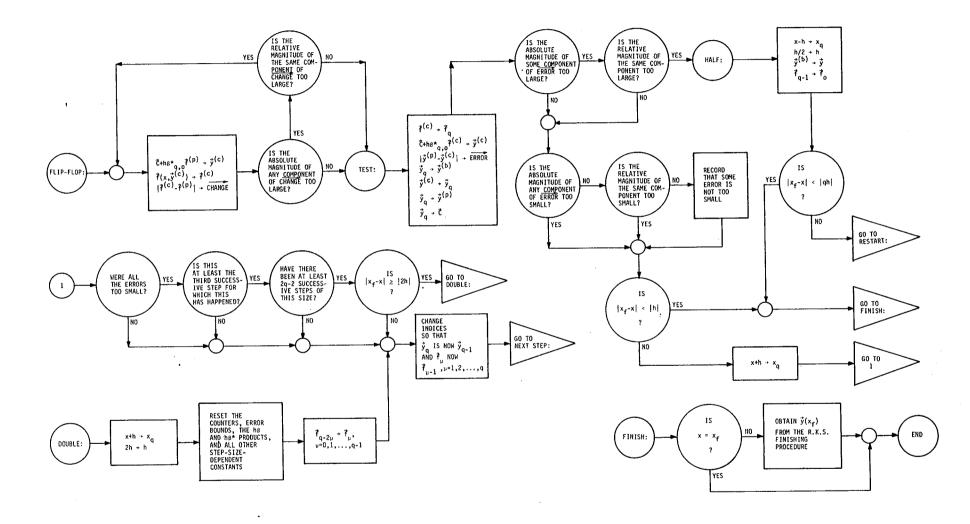


Figure 1 (Continued). Flow Diagram for the Adams Method.

A user interested in an efficient production program and desiring to eliminate the unnecessary moving of data resulting from the formerly separate arrays, as well as other easily discovered minor inefficiencies, should find the coordination of notation, identifiers, and labels between the preceding discussion and the following flow diagram and program listing sufficient to guide him in the task. Further, the coordination of the notation of this report with that of [5] should enable him to investigate the theory of the method of Adams with a minimum of effort expended on trivial translation.

The procedure ADAMS makes efficient use of B-5500 Algol under the restriction of generality with respect to order. However, in situations where only a few orders are needed, the running time can be decreased considerably by duplicating certain sections of the program for each order, using separate identifiers to replace much of the indexing and a switch to select the proper section of programming for a given order. Little investigation of the amount of saving achieved in this way has been done, and an evaluation of the potential gain should be profitable. This investigation might also include determination of the tradeoff between storage space and running time when a large number of orders is required.

Although the procedure ADAMS has now been tested on a wide range of equations, orders, and required accuracies with the existing step size controls, little has been done to determine the increases in efficiency to be obtained by varying the method of control and how the effects of such variation may depend upon order and required accuracy. The indication is that the existing controls produce considerably more accuracy than intended. This is particularly true when high accuracy is required at higher orders, where the penalty in running time is greatest and the largest variation in

step size has been observed. Repeated step size expansions and contractions of as much as 1024 to 1 have occurred. Even a slight relaxation of the requirements for expanding step size should produce dramatic decreases in running time. Determination of a way to do this safely should prove highly worthwhile. There is slight evidence that, while the error increases with increases in the factor GR at lower orders as might be expected intuitively, this effect apparently can reverse at higher orders. A study of this phenomenon could conceivably provide information useful in improving the efficiency of the step size controls.

OCEDURE ADAMS(N.XI	00000000
SCOEFF.START, SHANKS);	000100
LUE NOXIOXED	CV
AL XIXXFADADXX	000300
TEGER N. Q. RKSFNS, R	3
R. A.	50
DCFDUKE F.SHANKS:	9
TEGER PROCEDURE	~
	α: Ο
<i>Z</i>	0
DEFINE YIHY##YBHY##YFHY##POINTSH	10
NISE	dari,
ALL	
NITHKVALX(C2/C1))	ا نسان د لعان
STORY (NO XI)	<del>~</del> ;
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	220
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DOCK SECTION OF THE S	00024000
<u>.</u>	2
S	260
C ← ♡ ≯	270
_	280
+INTER!	290
ال السيا	300
<u>ئ</u> لىن	310
HB[MC]+B[MC]×H;	320
H8S[MU]+BS[MU]+BS[MU]×H3	330
	340
$\bigcirc$	350
10	360
	003700
NIS	003800
EALTIFCEAUTIFEATIIXCUIXCOMQPS;	00038000

```
ALLI YB[1]+YI[1]3
00061000
                                                                               f I X → X
00087000
                                                                E(NoXIoXIoEH[Oo+])}
00011000
                                                                          1SERU+1+01
00091000
                                                                              CS+CI?
00051000
                                                                                ENDE
00077000
00081000
                                                                   H←INTERVAL/C13
00021000
                                                                         CI+CI+CIE
00011000
                                                                               BECIN
00002000
                                                        MHIFE VB2(H)>DX OB C1<0 DD
00069000
                                                                         DX+ABS(DX);
00089000
                                                                  H+INTERVAL+XF-XI$
00029000
                                                                                (I+I)
00099000
                                                          GR+ADAMSCOEFF[QTIMES2+1])
00059000
                                                          BS0X+ADAMSCOEFF[OTIMES2];
00079000
                                                                                 ENDY
00063000
00029000
                                                                                       5
                                                         BS[WN] ← VD WWSCOELL[WN+0]}
00019000
                                                            B[MN]+ADAMSCOEFF[MU];
00009000
                                                                                BECIN
00065000
                                                                               UMJJA
00088000
                                                                    OLSWI + OLIWESS-11
00025000
                                                                        OLIMESS+0+01
00095000
                                                                        fI-0+ISONIWO
00022000
                                                                   CSW0b2+1\S*(0+2)}
00075000
                                                   BOOLEAN BGUOD, FLIPPED, TOOSMALL!
00023000
                     INTEGER ISSERVED COPCOMUNAULT, JZEROSOTZMISOMINUSISOTIMESZ!
00025000
                                                            CHANGE, C2MQP5, INTERVAL!
00015000
              REAL HAXACUAC2AGRAYCIABSQZAFHJIAFMUIAHBMUAM1DPAHBSMUAHBSQZAERRORA
00005000
                                                          EAL, ERUS ERL, HAL, HRLEO: NJJ
00067000
          REAL ARRAY FHIO: (2x0-2) DO: NJ DB BS DHB HBS [O:0-1] DC TPP YCO YD FF F C F E AU
00087000
                       LABEL RESTART, NEXTSTEP, FLIP, FLOP, TEST, DUBBLE, HALF, FINISH!
00024000
                                                                                END#1
00097000
00097000
                                                                               END
0000000
00064000
                                                      HRL[I] (ASS(ERL[I]/HBSQZ))
00045000
                                                      HAL[I] ← ABS(EAL[I] / HBSQZ);
00017000
                                              EBU[1] ← (EBU[1] ← EB[1]×CU)×C2MQP5
00007000
```

```
00080000
BGOOD+TRUE;
                                                                        00081000
RESTART: POINTS;
                                                                        00082000
C1+C1×MULT3
                                                                        00083000
C2+C2×MULT=Q3
                                                                        00084000
TF(J+JZERO=1)<OTHEN J+J+QT2M13
                                                                        00085000
RESET
                                                                        00086000
NEXTSTEP:X+XF=C2×H;
                                                                        00087000
ALLMU
                                                                        00088000
BEGIN
                                                                        00089000
  TF(J+J+1)=QT2M1 THEN J+0;
                                                                        00090000
  HBMU+HB[MU];
                                                                        00091000
  HBSMU+HBS[MU];
                                                                        00092000
  ALLI
                                                                        00093000
  REGIN
                                                                        00094000
    YP[I]+(FMUI+FH[J,I])×HBMU+YP[I];
                                                                        00095000
    C[I]+HBSMU×FMUI+C[I];
                                                                        00096000
                                                                        00097000
  FND3
                                                                        00098000
                                                                        00099000
ENDI
                                                                        00100000
F(NoXoYPoFP);
                                                                        00101000
FLIP: ALLI YC[I]+FP[I]×HBSQZ+C[I];
                                                                        00102000
F(N,X,YC,FC);
ALLI IF(CHANGE+ABS(FC[]]-FP[]))>HAL[]]THEN IF CHANGE>ABS(HRL[]]*FC[]]00103000
                                                                        00104000
THEN GO TO FLOP!
                                                                        00105000
FLIPPED+TRUE;
                                                                        00106000
GO TO TEST;
                                                                        00107000
FLOP:ALLI YC[I]+FC[I]×HBSQZ+C[I];
                                                                        00108000
F(N.X.YC.FP);
ALLI IF(CHANGE+ABS(FP[I]=FC[I]))>HAL[I]THEN IF CHANGE>ABS(HRL[I]*FP[I]00109000
                                                                        00110000
THEN GO TO FLIP
                                                                        00111000
FLIPPED+FALSEJ
                                                                        00112000
TEST: IF (J+J+1) =QT2M1 THEN J+0;
                                                                        00113000
TODSMALL+TRUE;
                                                                        00114000
ALLI
                                                                        00115000
BEGIN
                                                                        00116000
  FHJI+FH[J,I]+IF FLIPPED THEN FC[I]ELSE FP[I];
                                                                        00117000
  ERROR+ABS(YP[I]=(YCI+C[I]+YP[I]+(FHJI×HBSQZ+C[I])));
                                                                        00118000
  IF BGOOD THEN YD[I]+YCI ELSE YB[I]+YCI;
                                                                        00119000
  YCI+ABS(YCI);
```

```
00065100
                                                              IF C2≠OTHEN CALLOB!
                                                           X + X L = INTERVAL×(C2/C1) }
00085100
                                             IE NOT BGOOD THEN ALLI YBLIJ*YDLIJF
00025100
                                 FINISH: IF NOT FLIPPED THEN ALLI FC[1] FFE[1] }
00095100
00055100
                                                                   GO TO RESTARTS
                                           IL(CS+CS+CS+S°0)<0 THEN GD TO FINISH!
000124000
                                                                         CI+CI+CI)
00025100
                                                                          JZERO4JJ
00125000
                                                  HALF: IF( J+J-1) < OTHEN J+J+QT2M1;
00015100
                                                                   GO TO NEXISTEP!
00005100
                                              IF(J+(JZERJ+J)=1)<0THEN J+J+QT2M1;
00067100
                                                                              ENDY
00089100
00027100
00091100
                                                          ALLI FH(J,1) +FH(K,1);
00051100
                                                     IL(K+K=5)<01HEN K+K+OLSWI}
                                                     IF(JeJ=1)<0THEN JeJ+QT2M15
00011100
                                                                             BECIN
000143000
                                                  FOR MULISTEP 1UNTIL GMINUS1 DO
00142000
                                                                              K ← 11
0001#100
                                                                            RESELT
00000100
                                                                  CS+(CS-1*0)\S*0}
00068100
                                                              DOBBEE: CI+CI DIA St
00138000
00018100
                                                                   CO TO NEXISTEP?
00098100
                                       IF(JZERO+(J+JZERO)+1)=QT2M1 THEN JZERO+03
00032100
                                                                             £0→00
00012100
                                                                              END
00055100
                                                                 GO TO NEXTSTEP!
00135000
00012100
                                     IF(JZERO+(J+JZERO)+1)=QT2M1 THEW JZERO+OB
                       IL DC531HEN IE bC5015WI 1HEN IL CS511HEN CO 10 DOBBLEJ
00006100
                                                                        DC+DC+I}
00158000
00158000
                                                                             BECIN
                                                                  IE TOOSWALL THEW
00127000
00126000
                                       IF C221,0THEN C2+C2-1,0ELSE GD TO FINISH!
00122000
                                      IF BGOOD THEN BGOOD FFALSE ELSE BGOOD FTRUE!
                                                                          bC+bC+ll
00124000
                                                                              ENDY
00153000
00155000
                 IF ERROR>EAL(1)THEW IF ERROR>ERL(1)*YCI THEW TOOSMALL*FALSE!
00121000
                     IF ERROR>EAULIJTHEN IF ERROR>ERULIJ×YCI THEN GO TO HALF!
00150000
```

END 3

### B. The Method of Stetter, Gragg, and Butcher

#### 1. Description of the Method

Following is a discussion of a method for the numerical integration of ordinary differential equations described by J. C. Butcher [12] in a paper titled "A Modified Multistep Method for the Numerical Integration of Ordinary Differential Equations" which appeared in the January, 1965 issue of the Journal of the Association for Computing Machinery. In this paper, Butcher presents a modification to the multistep process such that for  $k \le 7$  (where k = 1 the number of steps) processes of order 2k + 1 are available.

A large number of possible multistep methods exist for the numerical integration of the differential equation

$$\frac{dy}{dx} = f(x,y), y(x_0) = y_0.$$
 (1-1)

Such methods are usually characterized by an integer k and a set of constants  $\alpha_1$ ,  $\alpha_2$  ---,  $\alpha_k$ ,  $\beta_0$ ,  $\beta_1$ , ---,  $\beta_k$ . A solution is first found for the variable y at a set of points  $x_1$ ,  $x_2$ , ---,  $x_{k-1}$ , (where  $x_1 = x_0 + ih$ ) and thereafter by the formula:

$$y_{n} = \alpha_{1} y_{n-1} + \alpha_{2} y_{n-2} + --- + \alpha_{k} y_{n-k}$$

$$+ h(\beta_{0} f_{n} + \beta_{1} f_{n-1} + --- + \beta_{k} f_{n-k})$$
(1-2)

for n = k, k + l, --- where  $y_i = y(x_i)$  and  $f_i = f(x_i, y_i)$ . Dahlquist [3] has shown that if the parameters  $\alpha$  and  $\beta$  are chosen under a condition of stability, the order of a method cannot exceed k + l (if k is odd) or k + 2 (if k is even).

A modification to this process is presented by Butcher which consists of the addition to the right-hand side of equation (1-2) of an extra term

h  $\beta$   $f_{n-\theta}$  where  $\beta$  and  $\theta$  are additional parameters to be chosen. The modified formula has the form:

$$y_{n} = \alpha_{1}y_{n-1} + \alpha_{2}y_{n-2} + \cdots + \alpha_{k}y_{n-k}$$

$$+ h \left(\beta f_{n-\theta} + \beta_{0}f_{n} + \beta_{1}f_{n-1} + \cdots + \beta_{k}f_{n-k}\right)$$
 (1-3)

A procedure for choosing the coefficients is presented by Butcher. The simplest stable processes are for k=1,2,3 with  $\theta=1/2$  and for k=4,5, 6 with  $\theta=1/3$ . A stable process also exists for k=7 with  $\theta=13/40$ .

The method for implementing the formulas is to estimate  $y_{n-\theta}$  and  $y_n$  using appropriate predictor formulas, then use these predicted values to evaluate the right-hand side of equation (1-3). The forms of the predictor formulas used are:

$$y_{n-\theta} = A_1 y_{n-1} + A_2 y_{n-2} + --- + A_k y_{n-k}$$

+ h 
$$(B_1f_{n-1} + B_2f_{n-2} + --- + B_kf_{n-k})$$
 (1-4)

$$y_n = a_1 y_{n-1} + a_2 y_{n-2} + --- + a_k y_{n-k}$$

+ h (b 
$$f_{n-\theta}$$
 +  $b_1 f_{n-1}$  +  $b_2 f_{n-2}$  + --- +  $b_k f_{n-k}$ ) (1-5)

To use this process,  $y_{n-\theta}$  is first estimated using equation (1-4). The value of the function is then determined for  $y_{n-\theta}$ , and these two results are used in equation (1-5) to determine a value for  $y_n$ . The value of the function is then determined for  $y_n$  and a final value is then estimated using equation (1-3).

### 2. The Computer Procedure

A single-precision ALGOL Procedure was written to implement the integration procedure described above on the Burroughs B-5500 Computer. The procedure was designed to be used with the driver program described elsewhere in this report, but it is conceivable that it could be used with other appropriate driver programs. The procedure was written to integrate a system of differential equations each of which has the form:

$$\frac{dy}{dx} = f(x,y), y(x_0) = y_0.$$

Since the integration procedure described by Butcher is a multistep process, it must at all times have a history of back points. The process is, therefore, not self starting; it must rely on some other process to develop the first k steps. The starting procedure used in this implementation is a basic Runge-Kutta procedure as modified by E. B. Shanks and is discussed in paragraph E of this chapter. The starting procedure is called at the beginning of an integration and whenever it is necessary to reduce the step-size.

The step-size control is based on the difference between a predictor and a corrector; the control allows for halving and doubling of the step-size only. Equation (1-5) is used as the predictor  $(y_{np})$  and equation (1-3) is considered to be the corrector  $(y_{nc})$ . An estimate of the magnitude of the error in a step is given by the absolute value of the difference in these two quantities. This is used in conjunction with a relative error term

ER and an absolute error term EA in the following manner: if

$$|\vec{y}_{np} - \vec{y}_{nc}| > (\vec{EA}) \left(\frac{DX}{XF - XI}\right)^{EX}$$

and

$$\left|\vec{y_{\rm np}} - \vec{y_{\rm nc}}\right| > \left|\vec{(ER)}(\vec{y_{\rm nc}})\right| \left(\frac{DX}{XF - XI}\right)^{EX}$$

then the step is rejected and the starting procedure is entered with the previous point and a step-size equal to half the old step-size. If

$$\left|\vec{y_{\text{np}}} - \vec{y_{\text{ne}}}\right| < (\vec{EA}) \left(\frac{DX}{XF - XI}\right)^{EX} \left(\frac{1}{2^{2k + 4}}\right)$$

 $\left| \vec{y_{\text{np}}} - \vec{y_{\text{nc}}} \right| < \left| (\vec{ER}) \left( \frac{DX}{XF - XI} \right)^{EX} (\vec{y_{\text{nc}}}) \right| \left( \frac{1}{2^{2k + 4}} \right)$ 

for three steps (without an intervening halving of the step-size) and if there is sufficient history of back points, then the step is accepted and the step-size is doubled. If neither the conditions for halving nor the conditions for doubling are met, then the step is accepted and the step-size remains constant. It is important to note that the above criteria must be satisfied for all corresponding components of the vector quantities before the conditions are considered to be met.

The method of ending the integration procedure is to run until the value of the independent variable plus the next step is either equal to or greater than the given final value i.e.

$$X + DX \ge XF$$
.

If it is exactly equal, then the procedure takes one more step and quits.

If X + DX > XF, then a special ending procedure is called to take the final step. This ending procedure is also a basic Runge-Kutta procedure as modified by E. B. Shanks. It is discussed in paragraph D of this chapter. The procedure call for the Butcher procedure must be as follows:

BUTCHER (N, XI, XF, K, EA, ER, DX, CON, FUNCTION, EX, RKC, START, SHANKS, YIV, RKSNF, RKSODR);

N - the number of dependent variables

XI - the initial value of the independent variable

XF - the final value of the independent variable

K - the number of steps to be used in the Butcher method

EA - the acceptable absolute error vector contained in an array of dimension N

ER - the acceptable relative error vector contained in an array of dimension N

DX - the suggested initial step-size

CON - the array row containing the Butcher constants required for the order of the method specified .

FUNCTION - the name of the user's function evaluation procedure

EX - the error exponent

RKC - the array containing the Runge-Kutta constants

SHANKS- the name of the ending procedure

START- the name of the starting procedure

YTV - the initial values of the dependent variable; upon exiting the Butcher procedure, this array will contain the final values of the dependent variables

RKSNF- the number of function evaluations in the Runge-Kutta Shanks procedure RKSODR - the order of the Runge-Kutta Shanks procedure

# 3. Flow Diagram and Program Listing

Figure 2 is the flow diagram for the method of Stetter, Gragg, and Butcher. A listing of the program is given at the end of this section.

### 4. Results and Conclusions

The following remarks will be directed to the problem of step-size control in the Butcher procedure. Although the method of step-size control, as described previously, was adequate for the purposes of this project, it is felt that some improvement is desirable. The difficulty observed was that in virtually all cases the accuracy achieved by the procedure was one to two orders of magnitude greater than the accuracy asked. For the third order Butcher process (k = 1), the step-size control method is completely unsatisfactory yielding long running times and accuracies as much as four times greater than those asked. The process in this case is essentially a third-order Runge-Kutta process. The equation used as a predictor in the step-size control scheme simply is not accurate enough in this case; this results in relatively large differences between the predictor and the corrector.

In order to improve the relation between the accuracy asked of the procedure and the accuracy achieved, it is desirable to study ways of improving the step-size control of the Butcher procedure. Such an improvement should also result in a faster running time for the method. One possible way of improving the step-size control is to use some form of two-step/one-step comparison. This could be accomplished in the Butcher process by using a predictor and corrector of the same order where the corrector uses alternate points of the history and a step-size twice as large as that of the predictor. The use of twice the step-size has the advantage of not requiring the recomputation of back points.

The investigation of new methods of step-size control should be done in double precision so that all of the orders of the Butcher process can be investigated. If single precision were used, only lowest orders of the process could be adequately investigated. This would not give a complete picture of the operation of the Butcher process.

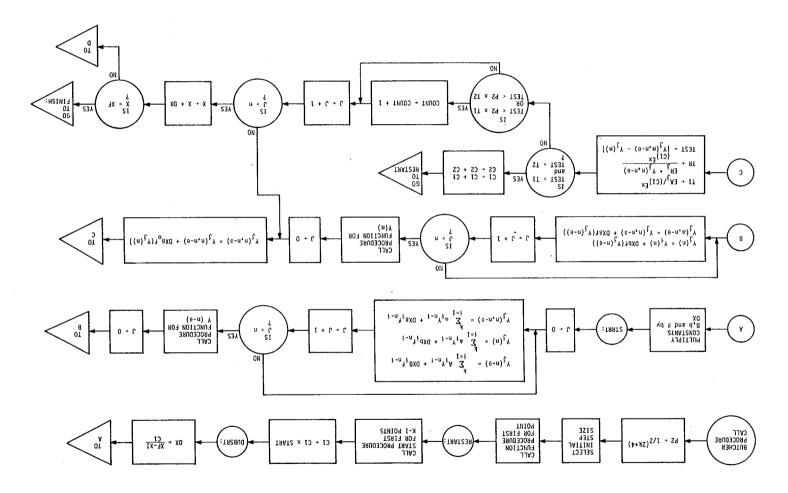


Figure 2. Flow Diagram for the Stetter-Gragg-Butcher Method.

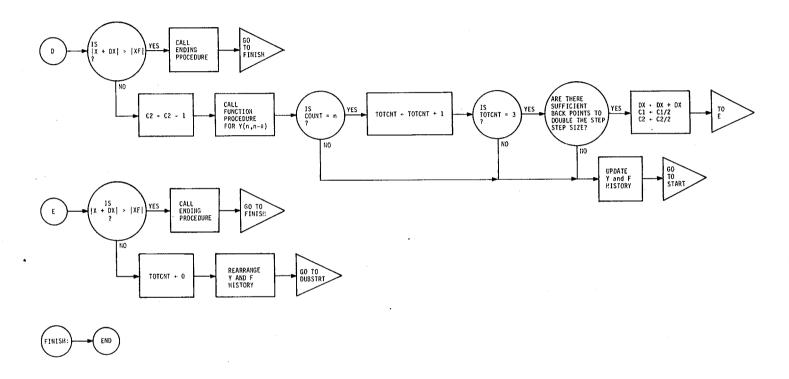


Figure 2 (Continued). Flow Diagram for the Stetter-Gragg-Butcher Method.

```
7
```

```
INTV < XF = XIJ
00038000
                                                                           KWI+K=I}
00038000
                                                                       K 2 5 ← ( 2 × K ) + S }
00035000
                                                                       K91+(0×K)+11
00036000
                                                                            KQ+QxK1
00035000
                                    IF K=10R K=20R K=3THEN OMT+0.5ELSE OMT+2/31
00034000
                                           FOR I & ISIEP TUNTIL N DO YEO ! 10 + YVV [1] .
00033000
                                                            REAL ARRAY REFAE[0:N];
00035000
                                                                     REAL XDXT, XDX;
0003E000
                                                             INTEGER KM3, J2, J3, J61
00000000
                                                                         REAL INTV
00053000
                                                              REAL UMTAKOAK61AK624
00088000
                                                                       INLEGER KMIS
00022000
                                                                   INTEGER COUNTERY
00058000
                                                                       INTEGER CYUJ
00052000
                                                            REAL ARRAY CUULO:3×K]
00054000
                                                                      LABEL DUBSRT
00023000
                                               INTEGER COUNTSTOTCHTSCYLLSONIS
00022000
                                                                     REAL P2, T1, T2,
00017000
                                                       LABEL STRRT, RESTART, FINISH,
000S000
                                          REAL ARRAY SUMYIP, SUMYP, SUMYC, FV1[0:N]J
00061000
                                                                      INTEGER CYL35
00081000
                                                       INTEGER INTOCALINDEXICIONS
00011000
             REAL DX1, COB, COLA, COLB, COGA, COG3, TEST, TEMPY, TEMPF, A1, A2, A3, C2,
00091000
                                                                          BEAL DX23
00051000
                                                                        BEAL SCINX!
00011000
                                                         REAL ARRAY YFF [0:16,0:N]
00013000
                                                                                 BECIN
00015000
00011000
                                                             REAL ARRAY CONSERSER[0] J
00001000
                                                                   REAL ARRAY RKCEOL
00060000
                                                                    REAL: XI.XF.DX.EXJ
00080000
                                                             INTEGER PROCEDURE STARTS
00020000
                                                           PROCEDURE FUNCTION, SHANKS!
00090000
                                                                          INTEGER N'KJ
00020000
                                                                INTEGER RKSNF, RKSOOR!
00000000
                                                                   REAL ARRAY YIVEOLF
 00000000
                                            VALUE N.XI.XF.K.DX.CON.EX.RKSNF.RKSODR!
0000000
                                                                   AIA BK 20E BK 2008)
 000010000
           PROCEDURE BUTCHER(N.XI.XF.K.EA.ER.DX.CON.FUNCTION.EX.RKC.START.SHANKS.
00000000
```

	0004000
. I	004200
2+013	004300
247	004400
پُ	004200
Y0+0}	004600
OTCNT+03	004700
UNCTIONCNOXIO	004800
ESTART & COUNTER + KM13	0004800
1+C1×(I+STAR1	EX0005000
RKSNF, RI	005100
2+C2×I=F	005200
YL+CYU)	005300
UBSRT	002400
MA+3XKM13	005200
DR J+OST	002600
EGIN	002500
2+2×J)	005800
00[J]+CON[J2+1]xDX	002300
00 [ J+1 ]+con[ J2+3]x	000900
00[J+2]+c0N[J2+5]xD	006100
:	006200
ON .	006300
C1 * FX **	006400
OR I+1ST	006500
N. G. I. N. H. G.	009900
الد	006700
ELIJ*ERLIJ/SC	006800
	006900
NUS	000700
1 + CUNEK 6 J×DX F	007100
2+CUN[K61]xUX	007200
34CON[K62]XDX}	007300
TRRI:XDXT + X+(	007400
	007500
OR IAISTEP TONTIL N DO	007600
OFCOLET TONILL KM1 U	001100
ן ≻ ט	006,000

	J3+3×J;	00080000
	J6+6×J}	00081000
	CDA+CDN[J6];	00082000
	COB+COO[J3];	00083000
	COLA+CON[J6+2];	00084000
	COLB+COO(J3+1];	00085000
	COGA+CON[J6+4];	00086000
	COGB+COO[J3+2];	00087000
	FOR I+1STEP 1UNTIL N DO	00088000
	BEGIN	00089000
	TEMPY+Y[CYL3,];	00090000
	TEMPF+F[CYL3,1];	00091000
	SUMYIP[I]+SUMYIP[I]+(CDA×TEMPY)+(COB×TEMPF);	00092000
	SUMYP[1]+SUMYP[1]+(COLA×TEMPY)+(COLB×TEMPF);	00093000
	SUMYC[I]+SUMYC[I]+(COGA×TEMPY)+(COGB×TEMPF);	00094000
		00095000
	END;	00096000
		00097000
	END;	00098000
	FUNCTION(N, XDXT, SUMYIP, FV1);	00099000
	FOR I+1STEP 1UNTIL N DO	00100000
4	BEGIN	00101000
•	TEMPF+FV1[I];	00102000
	SUMYP[I]+SUMYP[I]+(A1×TEMPF);	00103000
	SUMYC[I]+SUMYC[I]+(A2×TEMPF);	00104000
		00105000
	END#	00106000
	FUNCTION(N, XDX, SUMYP, FV1);	00107000
	CYL+(CYL+1)MOD 16;	00108000
	CYD+(CYL+KM1)MOD 163	00109000
	CDUNT+03	00110000
	FOR I+1STEP 1UNTIL N DO	00111000
	BEGIN	00112000
	TEMPY+SUMYC[1]+(A3×FV1[1]);	00113000
	T1 CAE[I];	00114000
	T2+ABS(RE[I]×TEMPY);	00115000
	TEST+ABS(TEMPY=SUMYP[I])}	00116000
	IF TEST>T1 AND TEST>T2 THEN	00117000
	BEGIN	00118000
	C2+C2+C23	00119000

```
35
```

```
00065100
                                                            ed in FINISH!
2HVNKS(N°X°XE°A[CAO°*]°ENNC11ON°KKSNE°KKSDDK°KKC°EX°EV°EK°DX)100128000
00025100
                                                                       BECIN
                                                                 IE CS<11HEN
00095100
00055100
                                                                    C1+C1\S)
00045100
                                                                    CS+CS\S}
00025100
                                                                  CONNIEK←01
00125000
                                                                         RECIN
00015100
                                                           IF COUNTERS2×K THEN
00005100
                                                                            BECIN
00067100
                                                                 IE 101CNIS31HEN
00084100
                                                                TOTCNI+TOTCNI+13
00014100
                                                                              BECTN
00097100
                                                                   IE COONLEN THEN
00057100
                                                 LONCIION(NEXELCADex ] DE[CADex ] ) }
00011100
                                                                               ENDE
000113000
00145000
                                                                   CO 10 LINISH:
               2HANK2(N»X»XE»X[CXQ»*]»ENNCIION»BK2NE°BK2ODB°BKC°EX°EP°EB°DX)}
00010100
00000100
                                                                              BECIN
                                                                       IL CS<ILHEN
00068100
00088100
                                                         IE CS=OIHEN GO TO FINISH!
00012100
                                                                      X + X L = (DX × CS) }
00098100
                                                                           C5+C5-13
                                                                               ENDY
00056100
000134000
00133000
                              IF TEST<P2×11 OR TEST<P2×12 THEN COUNT+COUNT+13
00135000
                                                                 ACCAD° I J + LEWBA3
000121000
                                                                             END
00002100
                                                                GO TO RESTART;
00150000
00128000
                                                                      CI+CI+CI)
                                                                           END)
0012100
00156000
00152000
                                                               CO LO LINIZHI
00124000
           2HVNKS(N>X>XF>X[CAO°*]>FUNCTION>RKSNF>RKSOOR>RKC>EX>EAFERDX)}
00153000
                                                                          BECIN
00155000
                                                                IL CS<KWI THEN
00151000
                                                          CAO¢(CAF+KWI)WOD 103
00150000
                                                           CAF CCAF + T2) WOD TOS
```

00161000 00161000 00162000 :L KM1 DG 00163000	00165000 00166000 00167000 00168000	00169000	00172000	00173000	00175000	00177000 00178000	00179000	00181000
END; TOTCNT+O; FOR I+1STEP 1UNTIL N DO FOR J+1STEP 1UNTIL BEGIN	<pre>CYL1+(CYD+16=J)MOD 16; CYL2+(CYO+16=(2×J))MOD 16; Y[CYL1*I]+Y[CYL2*I]; F[CYL1*I]+F[CYL2*I];</pre>	END	<u> </u>	END ;	END)	COUNTER COUNTER + 13	GO TO STRRT; FINISH:FOR I+1STEP 1 UNTIL N DO YIVEI3+YECYOPI	S END BUTCHER!

#### C. The Cowell Method

### Description of the Method

Cowell's method as described herein is a multistep predictor-corrector method for the numerical solution of the first-order vector differential equation

$$\vec{y}'(x) = \frac{d}{dx} \vec{y}(x) = \vec{f}(x, \vec{y}(x)), \vec{y}(x_0) = \vec{y}_0.$$
 (1-1)

A complete derivation and description of Cowell's method can be found in [ 9 ] and [ 18 ]; only the essential formulas are included here.

The following notation is adopted. Let q be an even positive integer, m=q/2, h be the step size (assumed to be constant over some set of calculations),

$$x_n = x_0 + nh$$
,  $\vec{y}_n = \vec{y}(x_n)$ , and  $\vec{f}_n = \vec{f}(x_n, \vec{y}_n)$ .

The predictor formula is

$$\vec{y}_{n} = h \left[ \delta^{-1} f_{n-\frac{1}{2}} + \sum_{j=0}^{q} P_{j} \vec{f}_{n-1-j} \right],$$
 (1-2)

The corrector formula is

$$\vec{y}_{n} = h \left[ \delta^{-1} f_{n-\frac{1}{2}} + \sum_{j=0}^{q} C_{j} \vec{f}_{n-j} \right], \qquad (1-3)$$

and the mid-range formula is

$$\vec{y}_{n} = h \left[ \delta^{-1} f_{n-\frac{1}{2}} + \sum_{j=0}^{q} M_{j} \vec{f}_{n+m-j} \right].$$
 (1-4)

The predictor formula gives  $\vec{y}_n$  in terms of  $\delta^{-1}f_{n-\frac{1}{2}}$  and the function values

at the previous q+l points; the corrector formula gives a new value of  $\vec{y}_n$  in terms of  $\delta^{-1}f_{n-\frac{1}{2}}$ , the old value of  $\vec{y}_n$ , and the function values at the previous q points; the mid-range formula gives a value of  $\vec{y}_n$  in terms of  $\delta^{-1}f_{n-\frac{1}{2}}$  and the function values at the q+l consecutive points centered around  $x_n$ .

The equation

$$\frac{1}{\delta^{-1}f_{n-\frac{1}{2}}} = \frac{1}{\delta^{-1}f_{n-1-\frac{1}{2}}} + \vec{f}_{n-1}$$
 (1-5)

completes the set of formulas necessary for the numerical solution of (1-1).

If it is assumed that

$$\{\vec{f}_i\}_{i=0}^q$$
 and  $\vec{y}_m$ 

have been obtained by some starting procedure, the mid-range formula (1-4) can be applied with n=m to obtain

$$\delta^{-1}f_{m-\frac{1}{2}}.$$

Equation (1-5) can then be applied m times to obtain

$$\delta^{-1}f_{q-\frac{1}{2}}$$
.

For each positive integer i

$$\frac{1}{\delta^{-1}f_{q+i-\frac{1}{2}}}$$

can be computed from

$$\delta^{-1}f_{q+i-1-\frac{1}{2}}$$

and  $\vec{f}_{q+i-1}$  using (1-5);  $\vec{y}_{q+i}$  can be computed using the predictor (1-2);  $\vec{f}_{q+i}$  can be computed from the predicted value;  $\vec{y}_{q+i}$  can be computed using the corrector (1-3);  $\vec{f}_{q+i}$  can be computed from the corrected value; if necessary, iteration can be resorted to, using (1-3), until the last two computed values of  $\vec{y}_{q+i}$  agree to sufficient accuracy. For any  $j \ge m$  a value of  $\vec{y}_{q+j-m}$  can be obtained from the mid-range formula (1-4) and compared with the value obtained from the predictor-corrector step. If the two values of  $\vec{y}_{q+j-m}$  are in sufficient agreement, the values up through  $\vec{y}_{q+j}$  are considered acceptable; if not,  $\vec{y}_{q+j-m}$  is considered the last acceptable value and all values beyond are rejected.

### 2. The Computer Program

The Cowell computer program is a Burroughs B-5500 ALGOL single-precision procedure whose declaration is as follows:

procedure Cowell (m, xi, xf, y, f, ea, er, p, dx, rksfn,

rksorder, rkscoeff, q, cowellcoeff, start, shanks);

value n, xi, xf, p, dx, rksfn, rksorder, q;

integer n, rksfn, rksorder, q;

real xi, xf, p, dx;

real array y, ea, er, rkscoeff, cowellcoeff [0];

procedure f, shanks;

integer procedure start;

The parameters of the procedure are defined as follows:

 $\underline{n}$  - the number of dependent variables in the vectors  $\overrightarrow{y}$  and  $\overrightarrow{f}$ 

 $\underline{xi}$  -  $x_0$ , the starting value of the independent variable x

 $\underline{xf}$  - the final value of the independent variable x

 $\underline{y}$  - the array in which  $\overrightarrow{y}_0 = \overrightarrow{y}(\underline{x}\underline{i})$  is located upon entry and in which  $\overrightarrow{y}(\underline{x}\underline{f})$  is located upon exit

 $\underline{\mathbf{f}}$  - the procedure which computes  $\overrightarrow{\mathbf{f}} = \overrightarrow{\mathbf{f}}(\mathbf{x}, \overrightarrow{\mathbf{y}})$ 

ea - the array containing the absolute error vector

er - the array containing the relative error vector

 $\underline{p}$  - the exponent used in step size control

<u>rksfn</u> - the number of function evaluations used in the Runge-Kutta-Shanks starting and closing procedures

rksorder - the order of the Runge-Kutta-Shanks closing procedure

rkscoeff - the array containing the Runge-Kutta-Shanks coefficients
for the starting and closing procedures.

 $\underline{\mathbf{q}}$  - the even integer used in describing Cowell's method

cowellcoeff - the array containing the Cowell coefficients

start - the starting procedure

shanks - the closing procedure.

The procedure performs the numerical integration of (1-1) from  $x = \underline{x}\underline{i}$  to  $x = \underline{x}\underline{f}$ . The step size h used is always the length of the interval  $\underline{x}\underline{f} - \underline{x}\underline{i}$  divided by a power of 2 in order to avoid error building in the independent variable two counters,  $\underline{c}\underline{l}$  and  $\underline{c}\underline{c}\underline{l}$  are kept.  $\underline{c}\underline{l}$  is always a positive, integral power of 2, and  $\underline{h} = (\underline{x}\underline{f} - \underline{x}\underline{i})/\underline{c}\underline{l}$ .  $\underline{c}\underline{c}$  is the number of steps necessary to step from the present x to  $\underline{x}\underline{f}$  using the current step size h. Initially  $\underline{c}\underline{c}\underline{l} = \underline{c}\underline{l}$ ; as each step is taken  $\underline{c}\underline{c}\underline{l}$  is decremented by one and the present value of x is

computed by  $\underline{x} = \underline{xf} - h \underline{c2}$ . If h is halved,  $\underline{c1}$  and  $\underline{c2}$  are doubled; if h is doubled,  $\underline{c1}$  and  $\underline{c2}$  are halved. Hence  $\underline{c2}$  need not be integral.

The error vectors  $\overrightarrow{ea}$  and  $\overrightarrow{er}$ , like  $\overrightarrow{y}$ , have n components. (Although the base of the arrays  $\underline{y}$ ,  $\underline{ea}$ , and  $\underline{er}$  is zero, the n components are placed in positions 1, 2, ..., n of the arrays.) The procedure's error control attempts to guarantee that, in integrating from xi to xf, each component of  $\overrightarrow{y}$  will not be in absolute error more than the corresponding component of  $\overrightarrow{ea}$  and will not be in relative error more than the corresponding component of  $\overrightarrow{er}$ . At each step, the procedure requires that for each i,  $1 \le i \le n$ , either the absolute error in y [i] does not exceed ea [i]/(cl<sup>P</sup>) or the relative error in y [i] does not exceed er [i]/(cl<sup>P</sup>).

If p=1 and  $\overrightarrow{er}=0$  then the accumulated error in any component of  $\overrightarrow{y}$  cannot exceed the corresponding component of  $\overrightarrow{ea}$ . If the error is assumed to accumulate randomly as the square root of the number of steps,  $p=\frac{1}{2}$  and  $\overrightarrow{er}=0$  will cause the accumulated error in any component of  $\overrightarrow{y}$  to be approximately the corresponding component of  $\overrightarrow{ea}$ .

If p=1 and  $\vec{ea}=0$  then the accumulated error in any component of  $\vec{y}$  cannot exceed the corresponding component of  $\vec{er}$  times the largest value assumed by that component of  $\vec{y}$  during the integration. If the error is assumed to accumulate randomly as the square root of the number of steps,  $p=\frac{1}{2}$  and  $\vec{ea}=0$  will cause the accumulated error in any component of  $\vec{y}$  to be approximately the corresponding component of  $\vec{er}$  times some average value assumed by that component of  $\vec{y}$  during the integration.

The procedure  $\underline{f}$  which computes  $\overrightarrow{f} = \overrightarrow{f}$  (x,y) has the following declaration:

procedure f(n, x, yv, fv);

value n;

integer n;

real x;

real array yv, fv [0];

The parameters of the procedure  $\underline{f}$  are defined as follows:

 $\underline{n}$  - the number of dependent variables in the vectors  $\overrightarrow{y}$  and  $\overrightarrow{f}$ 

 $\underline{x}$  - the value of the independent variable

 $\underline{yv}$  - the array in which  $\overrightarrow{y}$  is stored

fv - the array in which  $\overrightarrow{f}$  is stored after computation

The procedure <u>start</u> is the general multistep method starting procedure described in paragraph E of this chapter. The procedure <u>shanks</u> is the Runge-Kutta-Shanks integration procedure described in paragraph D of this chapter. The coefficient array <u>rkscoeff</u> contains the Runge-Kutta-Shanks coefficients in the order required by the procedures <u>start</u> and <u>shanks</u>. The number of function evaluations <u>rksfn</u> is required by both <u>start</u> and <u>shanks</u>; the order <u>rksorder</u> is required by <u>shanks</u>.

The array <u>cowellcoeff</u> contains the coefficients of (1-2), (1-3), and (1-4) in the order  $P_0$ ,  $P_1$ , . . . ,  $P_q$ ,  $C_0$ ,  $C_i$ , . . . ,  $C_q$ ,  $M_0$ ,  $M_1$ , . . . ,  $M_q$ ;  $P_0$  is in the zero position of the array.

The suggested initial step size  $\underline{dx}$  is optional. The procedure first sets  $\underline{cl} = 2$  and doubles  $\underline{cl}$  until  $\underline{cl} \ge q$ . If  $\underline{dx} = 0$  or  $\underline{dx} \ne 0$  and  $\underline{h} \le |\underline{dx}|$  then  $\underline{cl}$  is left alone. Otherwise,  $\underline{cl}$  is doubled until  $\underline{h} \le |\underline{dx}|$ . The integration now begins.

$$\vec{f}_0 = \vec{f}(x_0, \vec{y}_0)$$

is computed. The start procedure is called to obtain

$$\left\{f_{i}\right\}_{i=1}^{q}$$
 ,  $\vec{y}_{m}$ ,  $\vec{y}_{q}$  and  $\mathbf{x}_{q}$ .

cl and c2 are adjusted if h was changed by the start procedure. c2 is decremented by q since q steps took place in the start procedure. If c2 < m, closing takes place. Otherwise,

$$\frac{1}{\delta^{-1}f_{m-\frac{1}{2}}}$$

is calculated from

$$\left\{f_{i}\right\}_{i=0}^{q}$$

and  $\vec{y}_m$  using the mid-range formula (1-4). m applications of (1-5) yield

$$\delta^{-1}$$
  $q^{-\frac{1}{2}}$ 

and n is set equal to q.

For  $1 \le i \le m$  the following set of steps takes place. c2 is decremented by 1, and  $\boldsymbol{x}_{n+i}$  is calculated.

$$\frac{->}{\delta^{-1}} f_{n+i-\frac{1}{2}}$$

is calculated from

$$\delta^{-1}f_{n+i-1-\frac{1}{2}}$$

and  $\vec{f}_{n+i-1}$  using (1-5).  $\vec{y}_{n+i}$  is calculated using the predictor (1-2), and

 $\vec{f}_{n+i}$  is calculated.  $\vec{y}_{n+i}$  is next calculated using the corrector (1-3), and  $\vec{f}_{n+i}$  is again calculated. Let  $\vec{v}$  be the vector which is the absolute value of the difference between the last two calculated values of  $\vec{y}_{n+i}$ . Each component of  $\vec{v}$  is compared with the corresponding component of  $\vec{ea}/(10 \cdot cl^p)$  for absolute error and with the product of the corresponding components of  $\vec{er}/(10 \cdot cl^p)$  and the last calculated value of  $\vec{y}_{n+i}$  for relative error. If any component of  $\vec{v}$  exceeds in both the absolute and the relative error tests, the steps which calculate  $\vec{y}_{n+i}$  using the corrector (1-3), calculate  $\vec{f}_{n+i}$  from the value of  $\vec{y}_{n+i}$ , and which test the last two calculated values of  $\vec{y}_{n+i}$  are repeated. When each component of  $\vec{v}$  does not exceed in either the absolute or the relative error test, the last values of  $\vec{y}_{n+i}$  are retained.

The mid-range formula (1-4) is now used to calculate a new value of  $\vec{y}_n$  from

$$\left\{f_{n+i}\right\}_{i=-m}^{m}$$

and

$$\delta^{-1} f_{n-\frac{1}{2}}$$

Let  $\vec{v}$  be the vector which is the absolute value of the differences between the new value of  $\vec{y}_n$  and the previously calculated value of  $\vec{y}_n$ . If sufficient history is available for doubling the step size, i.e., n>q+m, each component of  $\vec{v}$  is compared with the corresponding component of  $\vec{ea}/(10 \cdot \text{cl}^p \cdot 2^{q+3})$  for absolute error and with the product of the corresponding components of  $\vec{er}/(10 \cdot \text{cl}^p \cdot 2^{q+3})$  and the new value of  $\vec{y}_n$  for relative error.

If each component of  $\vec{v}$  does not exceed in either the absolute or the relative error tests, the last m steps are accepted, cl and c2 are halved, and the step size is doubled. If c2 < m, closing takes place. Otherwise

$$\{f_i\}$$
 q i=0

becomes

$$\left\{\vec{f}_{n-m+2i}\right\} \ \ \stackrel{q}{\underset{i=0}{\text{i=0}}} \ ,$$

 $\vec{y}_m$  becomes  $\vec{y}_{n-m}$ ,  $\vec{y}_q$  becomes  $\vec{y}_{n+m}$ ,  $x_q$  becomes  $x_{n+m}$ , and, as if the starting procedure had calculated these values, control returns to the step where

$$\delta^{-1}f_{m-\frac{1}{2}}$$

is calculated using the mid-range formula (1-4).

If any component of  $\vec{v}$  exceeds in both the absolute and the relative error tests, this component and each untested component is compared with the corresponding component of  $\vec{ea}/(10 \cdot \text{cl}^p)$  for absolute error and with the product of the corresponding components of  $\vec{er}/(10 \cdot \text{cl}^p)$  and the new value of  $\vec{v}$  for relative error. If each component of  $\vec{v}$  does not exceed in either the absolute or the relative error test, the last m steps are accepted and the step size remains unchanged. If c2 < m, closing takes place. Otherwise, n becomes n + m and control returns to the steps which calculate

$$\left\{ \mathbf{y}_{\mathrm{n+i}} \right\} \begin{array}{c} \mathbf{m} \\ \mathrm{i=l} \end{array}$$
 .

If any component of  $\overrightarrow{v}$  exceeds in both the absolute and the relative error tests,

the last m steps are rejected, c2 is incremented by m, c1 and c2 are doubled, and the step size is halved.  $\vec{f}_0$  becomes  $\vec{f}_n$ ,  $\vec{y}_0$  becomes  $\vec{y}_n$ ,  $\vec{x}_0$  becomes  $\vec{x}_n$ , and control is returned to the step which calls the start procedure.

If sufficient history is not available for doubling, control transfers as if the first component of  $\vec{v}$  exceeded both the first component of  $\vec{ea}/(10 \cdot \text{cl}^p \cdot 2^{q+3})$  and the product of the first components of  $\vec{er}/(10 \cdot \text{cl}^p \cdot 2^{q+3})$  with the first component of the new value of  $\vec{y}_n$ .

Closing takes place whenever m steps at the present step size would carry the integration beyond xf, i.e., whenever c2 < m. If c2 > 0, the Runge-Kutta-Shanks procedure is used to integrate from the present value of x to xf; if c2 = 0, the present value of x is xf. In either case, the integration is now complete.

Several efficiency measures are employed in the program. First, the coefficients

$$\left\{ P_{j}\right\} \stackrel{q}{j=0}$$
,

$$\left\{ c_{j}\right\} _{j=0}^{q}$$
 ,

and

$$\left\{M_{\mathbf{j}}\right\} \stackrel{\mathbf{q}}{\mathbf{j}=0}$$

are multiplied by the step size h and stored as multiplied until the step size changes. Second, the vectors  $\vec{ea}/(10 \cdot \text{cl}^p)$ ,  $\vec{er}/(10 \cdot \text{cl}^p)$ ,  $\vec{ea}/(10 \cdot \text{cl}^p \cdot 2^{q+3})$ , and  $\vec{er}/(10 \cdot \text{cl}^p \cdot 2^{q+3})$  are calculated from  $\vec{ea}$  and  $\vec{er}$  and stored as calculated until the step size changes. Third, the corrector

partial sum

$$h\delta^{-1}f_{n-\frac{1}{2}} + h\sum_{j=1}^{q} C_{j}f_{j}$$

is computed and stored at each step; successive applications of the corrector only require adding  $h \cdot C_0 \cdot f_n$  to obtain  $\vec{y}_n$ . Fourth, during applications of the corrector, two arrays are used to store the last two calculated values of  $\vec{y}_n$ ; a flag is used to mark the last calculated value so that the next value is placed in the unflagged array and the flag is switched. This avoids transfer from array to array as successive corrector iterates are computed. Fifth, cyclic indexing is used to avoid moving the function value history after each step or set of steps unless doubling takes place.

One unusual condition can result. If, during any step taken in computing

$$\left\{ \vec{y}_{n+i} \right\}_{i=1}^{m},$$

the number of times through the corrector exceeds eight, control transfers as if the set of m steps has been completed and rejected, i.e., a step size halving was called for with a restart beginning at  $\vec{y}_n$ .

## 3. Flow Diagram and Program Listing

Figure 3 is the flow diagram for the Cowell method. The program listing follows at the end of this section.

## 4. Results and Conclusions

The first important conclusion concerns the error control. The specified tolerances for absolute and relative error are handled vectorially to allow for systems in which the units of the various dependent variables are not the same. Such systems arise in physics, for example, from reduction of second order equations of motion in two dimensions to a first order system in

which two variables are positions and two variables are velocities. More important, however, is the requirement at each step that the error in each variable not exceed the specified tolerances divided by  ${\rm cl}^p$ , where  $0 \le p \le 1$ . If p=0, conventional vectorial error control results. If  $p \ne 0$ , however, an interesting phenomenon occurs. As the step size decreases, higher accuracy is required; as the step size increases, less accuracy is required. Hence, halving is often required sooner after a previous halving than when p=0, and halving immediately after doubling is less frequent since the increase in error due to doubling is accompanied by a decrease in accuracy required.

One major result of this error control is the linearity of error obtained as a function of error asked. Earlier experiments [18] with p=0 showed that dividing the asked error by ten sometimes had little or no effect on the error obtained; dividing the error asked by two sometimes decreased the error obtained by a factor of ten. Present experiments with  $p=\frac{1}{2}$  show that multiplication of the error asked by a constant usually causes the error obtained to be multiplied by the same constant.

Division of the asked error tolerances by 10 . cl<sup>p</sup> rather than cl<sup>p</sup> was determined experimentally to be necessary in order to assure that the error at each step be held to its desired value. This seems to be a peculiarity of the mid-range formula type of error estimation; namely, that the actual error after each set of m steps can be as much as ten times as large as the estimate given by the mid-range test.

Doubling occurs when the estimated error is less than the asked error tolerances divided by 10  $\cdot$  cl<sup>p</sup>  $\cdot$  2<sup>q+3</sup>; hence, the doubling criteria are the accepting criteria divided by 2<sup>q+3</sup>. This factor was also chosen experimentally,

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					•		

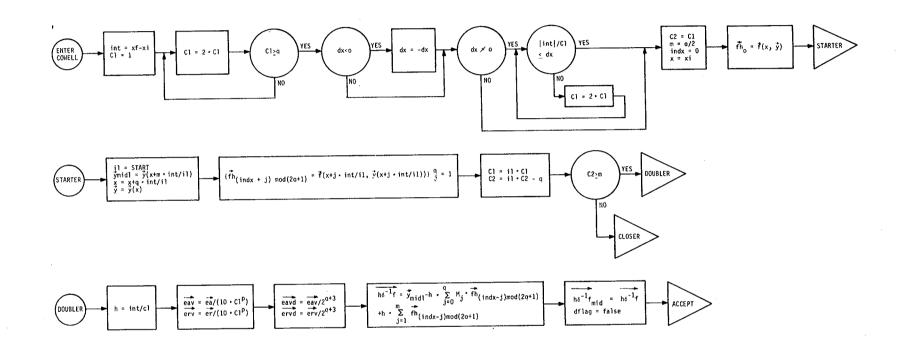


Figure 3. Flow Diagram for the Cowell Method.

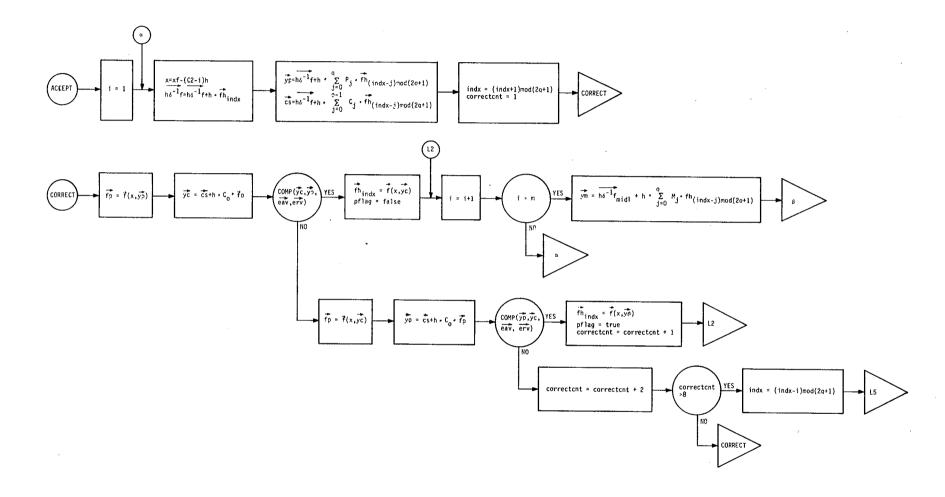


Figure 3 (Continued). Flow Diagram for the Cowell Method.

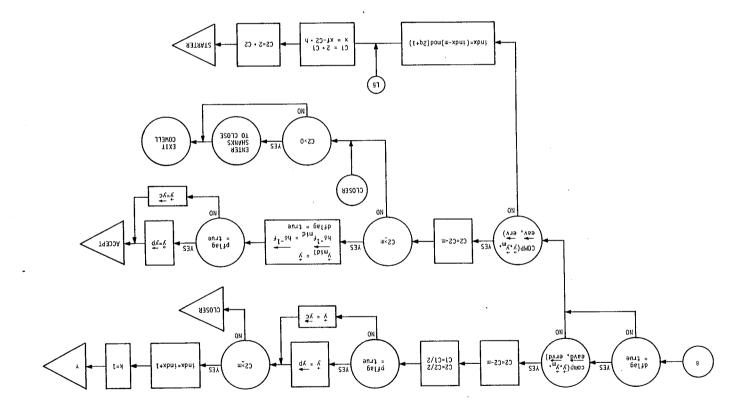


Figure 3 (Continued). Flow Diagram for the Cowell Method.

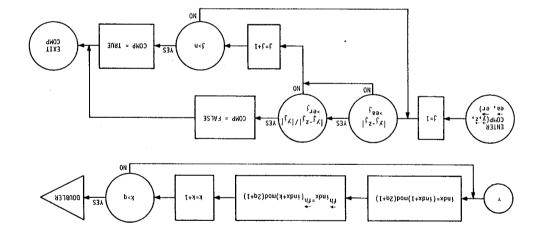


Figure 3 (Continued). Flow Diagram for the Cowell Method.

and it is the same factor that was determined in earlier experiments with p = 0 [18].

One other consequence of the present error control is the limitation of accuracy obtainable with a single precision program. When the relative estimated error is required to be less than  $10^{-11}$  for doubling to occur, doubling is almost precluded since the computer can only carry eleven to twelve decimal digits. Under such conditions the number of steps increases enormously, and the program is virtually useless. For p=0 and variables of order of magnitude one, this situation occurs when the error asked divided by  $10 \cdot 2^{q+3}$  is about  $10^{-11}$ ; however, with  $p \neq 0$ , this situation occurs when the step size is such that the error asked divided by  $10 \cdot c1^p \cdot 2^{q+3}$  is about  $10^{-11}$ . Thus the smallest allowable asked error is reduced as p approaches one.

Since the even integer q is also involved in the calculation of the smallest allowable asked error, it becomes apparent that the smallest allowable asked error can be asked with small q, yet the larger values of q offer their biggest advantage at higher asked accuracies. Results show that best single precision results tend to come from runs with q = 4 and q = 6 at the asked accuracies which are reasonable for single precision; earlier experiments with double precision asking higher accuracies [18] showed that best results came from higher values of q.

The matching of the order of the start procedure with the order of the Cowell method was somewhat difficult due to the limitation on accuracy asked. The (4,4) Shanks formula seemed to give best results for q=4, at all accuracies and best results for q=6 at larger asked errors; the (5,5) Shanks formula seemed to give best results for q=6 at smaller or asked error. These results were not extensive enough to be conclusive, however.

Corrector convergence can become a problem under two conditions. First, the Runge-Kutta-Shanks formulas can take much larger steps than the Cowell method at lower asked accuracies. The step size chosen by the start procedure can be large enough so that the Cowell corrector will not converge, yet the steps are accurate enough as Runge-Kutta-Shanks steps. Second, in rapidly approaching a singularity the step size could suddenly become too large for Cowell corrector convergence, for step size control is only exercised after each m steps. The corrector counter was required to protect against the corrector not converging; a halving is called for whenever more than eight times through the corrector become necessary.

A final result concerns second order systems. Cowell's method was originally a pair of predictor and corrector formulas to be used to compute the positions as well as the velocities directly from the function value history. The predictor and corrector to compute the positions was of one higher order than the corresponding velocity formulas. Earlier experiments [18] were made using this type of approach. Present experiments required the second order system to be reduced to a first order system; the predictor and corrector are simply the velocity formulas. Both earlier and present experiments show the positions to be more accurate than the velocities; hence only time, not accuracy, is lost when a second order system must be solved as a first order system.

```
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           SIRRIERSCI SECII SESIRRICIVOXIOXEDCIDERDERDEDOXONOLDENDENDIDIDINUXD
00088000
                                                               F(NoxaveH[Oakl))
00035000
                                                                         ¶ IX±8 X
00098000
                                                                       INDX 8=0 }
00032000
                                                          DEACTUR 8=200 *(Q +3)
00034000
                                                                 1 00 190=: 1901
00033000
                                                                     1 14 0=: 140
00035000
                                                                     I - WES INW
00011000
                                                                    W #= O DIA S }
00000000
                                                                        CS t=CI ?
00020000
                                                                            END 1
00088000
                                                                            0N3
00075000
                                                                     GO TO L1
00092000
                                                               c1 := c1 + c1 }
000S2000
                                                                         BECIN
00024000
                                                    List ABSCINT)/C1 >DX THEN
00083000
                                                                            BECIN
00022000
                                                                   IE DX ¥O THEN
00057000
                                                        IL DX <0 THEN DX ===DX }
                                                        IL CI <0 THEN GO TO J
00002000
00061000
                                                                 f 10+ 10=: 10:07
00081000
                                                                         CI tal 1
00011000
                                                                   INI :=XL =XI }
00091000
                LABEL LO⊅L1⊅L2⊅L3⊅L4⊅L5⊅STAKTER⊅DUUBLEK≯ACCEPT⊅CORKECT⊅CLOSER}
00012000
                                     DEAVD. ERVD[0:N] PPCOEFF CCOEFF MCOEFF[0:0];
BEAL ARRAY FHLOSG 4008N) PYMID127PYC2MACSSPPPHDM1F9HDM1FMID2EAVERV 00014000
00013000
                                                           BOOLEAN DFLAG, PFLAG 3
00015000
                                    REAL INTOC20DFACTOROXAHOT10T20T30T40T50T6 &
00011000
                                                            INTEGER CORRECTOR 3
                            INTEGER CLOMOMMIOPPIOPLOPIONOXO[1012013010JoKoCYI V
00001000
00060000
                                                                              BECIN
00080000
00020000
                                                         INTEGER PROCEDURE START 3
00090000
                                                              PROCEDURE FISHANKS }
                                      REAL ARRAY YVEAVERARKSCOEFFACOWELLCOEFF[0];
00050000
00000000
                                                                 REAL XI,XF,P,DX ;
00060000
                                                      INTEGER NORKSFNORMSORDEROG 3
0000000
                                             VALUE N.XI.XF.P.DX.RKSFN.RKSORDER.O 3
00010000
                                                        COMELLCOEFF, START, SHANKS);
00000000
              HUCCEDOME COMETE(N⊅XIDXEDÁDEDEVEBBBDDXDMK2ENDMK2OBDEBDBK2COELEDOD
```

```
TQP1,1,P,RKSFN,RKSCDEFF))xC1 }
                                                                          00040000
C2 8=C2 ×I1 =Q 3
                                                                          00041000
INDX :=(INDX +Q)MDD TQP1 ;
                                                                          00042000
IF C2 <M THEN GO TO CLOSER 3
                                                                          00043000
DOUBLERSH := INT /C1 3
                                                                          00044000
FOR K 8=0 STEP 1 UNTIL Q DO
                                                                          00045000
BEGIN
                                                                          00046000
  PCDEFFEK3 * = COWELLCOEFF(K) × H ;
                                                                          00047000
  CCOEFFIK] := COWELLCOEFFII1 := K + QP1] × H ;
                                                                          00048000
  MCOEFF(K) 8 = COWELLCOEFF(I1 +QP1)×H
                                                                          00049000
END ;
                                                                          00050000
T1 = (C1 + P) \times 10.0 
                                                                          00051000
FOR J := 1 STEP 1 UNTIL N DO
                                                                          00052000
BEGIN
                                                                          00053000
  EAVD[J]:=(EAV[J]:=EA[J]/T1)/DFACTOR;
                                                                          00054000
  ERVD[J]:=(ERV[J]:=ERFJ]/T1)/DFACTOR
                                                                          00055000
END 3
                                                                          00056000
T1 #=MCDEFF[0];
                                                                          00057000
FOR J :=1 STEP 1 UNTIL N DO HDM1F[J]:=YMID1[J]=FH[INDX,J]×T1 }
                                                                          00058000
CYI := INDX +TQP1 ;
                                                                          00059000
I3 :=CYI -OP1 ;
                                                                          00060000
FOR K :=1 STEP 1 UNTIL M DO
                                                                          00061000
BEGIN .
                                                                          00062000
  I1 := (CYI =K)MOD TQP1 ;
                                                                          00063000
  I2 #=(I3 +K)MOD TQP1 #
                                                                          00064000
  T1 :=MCDEFF(K)=H ;
                                                                          00065000
  T2 :=MCDEFF[QP1 =K];
                                                                          00066000
  FOR J == 1 STEP 1 UNTIL N DO HDM1F[J]=HDM1F[J]=FH[I1,J]×T1 =FH[I2,J]00067000
  xT2
                                                                          00068000
END 3
                                                                          00069000
FOR J :=1 STEP 1 UNTIL N DO HDM1FMID[J]:=HDM1F[J];
                                                                          00070000
DFLAG :=FALSE ;
                                                                          00071000
ACCEPT:FOR I := 1 STEP 1 UNTIL M DO
                                                                          00072000
BEGIN
                                                                          00073000
  CYI :=(INDX :=(INDX +1)MOD TQP1)+TQP1 ;
                                                                          00074000
  X := XF = (C2 = I) \times H 
                                                                          00075000
  I1 :=(CYI ~1)MOD TQP1 ;
                                                                          00076000
  T1 :=PCOEFF[0];
                                                                          00077000
  T2 :=CCOEFF[1];
                                                                          00078000
  FOR J := 1 STEP 1 UNTIL N DO
                                                                          00079000
```

-	00800
YP[J]:=(T4 :=(	00810
CS[J]:=14 +T2	00820
2	00830
-0P1 ;	00840
OR K :=2 STEP	00820
EGIN	00860
1 *=(CYI "K)MOD T	00870
2 SH(I3 +K)MOD TO	00880
1 SEPCOEFFIK	06800
2 *=CCOEFFIK	00600
3 **PCOEFFEG *K1	00910
4 SECCOEFFIGP1 =K1	00650
DR J 1=1 STE	06600
ZISE	00940
P[J] t=YP[J]+T1 x(T5 t=FH	00620
CS[J] # CS[J] + T2 × T5 + T4 × T	09600
END	02600
•• CZ	08600
1 :=(CY1 -@)MOD	06600
2 == (CYI = QP1)M	01000
1 :=PCOEFF[0 -1]	01010
2 taccoeff[0];	01020
3 ##PCOEFFE@1#	01030
OR J :=1 STEP	01040
N I 5 H	01050
YPEJJ:#YPEJJ+T! xC	01060
CS[J]##CS[J]#T	01070
TON STREET	01080
2 THCCORFF[0]3	01070
NO XOYPOPP); STEP 1 UNTIL	00111000
UJ))*YP[UJ)>>EAV[U]THEN	01130
EGIN	01140
<b>⊢</b>	01150
EGI	01160
OR J #= J +	01170
F(NexetCefP)} FOR J 181 STEP 1 INTIL N OO 15 (11 184ABS//13 82(YP[J]84CS[J]+10	$\circ$

```
00121000
                              00122000
                                                         00124000
                                                                                                                          00129000
                                            00123000
                                                                     00125000
                                                                                   00126000
                                                                                                 00127000
                                                                                                              00128000
                                                                                                                                        00130000
                                                                                                                                                     00131000
                                                                                                                                                                  00132000
                                                                                                                                                                                00133000
                                                                                                                                                                                            00134000
                                                                                                                                                                                                          00135000
                                                                                                                                                                                                                      00136000
                                                                                                                                                                                                                                   00137000
                                                                                                                                                                                                                                                 00138000
                                                                                                                                                                                                                                                              00139000
                                                                                                                                                                                                                                                                            00140000
                                                                                                                                                                                                                                                                                         00141000
                                                                                                                                                                                                                                                                                                      00142000
                                                                                                                                                                                                                                                                                                                   00143000
                                                                                                                                                                                                                                                                                                                                 00144000
                                                                                                                                                                                                                                                                                                                                               00145000
                                                                                                                                                                                                                                                                                                                                                            00146000
                                                                                                                                                                                                                                                                                                                                                                          00147000
                                                                                                                                                                                                                                                                                                                                                                                      00148000
                                                                                                                                                                                                                                                                                                                                                                                                   00149000
                                                                                                                                                                                                                                                                                                                                                                                                                00150000
                                                                                                                                                                                                                                                                                                                                                                                                                             00151000
                                                                                                                                                                                                                                                                                                                                                                                                                                          00152000
                                                                                                                                                                                                                                                                                                                                                                                                                                                       00153000
                                                                                                                                                                                                                                                                                                                                                                                                                                                                   00154000
                                                                                                                                                                                                                                                                                                                                                                                                                                                                                 00155000
                                                                                                                                                                                                                                                                                                                                                                                                                                                                                               00156000
                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                            00157000
                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                          00158000
                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                       (T2 1=ABS((T3 1=Y[J])=YM[J])>EAVD[J
                                                                                                                                                                                                                                                                                                                                                                                                                                                                  DO YMIJJI=YMIJJ+T1 xFHIII>JJ+T2 xFHII2>JJ
                                                       N DO YP[J] # CS[J] + T2 xFP[J]
                                                                                                                                                                                                                                                                                                                                                          N DO YM[J]1 = HDM1FMID[J] + T1 XFH[I1 + J]
                                                      FOR J := J +1 STEP 1 UNTIL
                                                                                                          INDX 1=(CYI -I)MOD TOP1
                                                                   CORRECTONT *=CORRECTONT
XFP[J]))-YC[J])>EAV[J]THEN
                           >ERVE J3XABS(T3)THEN
                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                        <u>...</u>
                                                                               F CORRECTONT >8 THEN
                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                        00
                                                                                                                                                                                                                   CORRECTONT : #CORRECTONT
                                                                                                                                                                                                                                                                                                                                                                                   FOR K := 0 STEP 1 UNTIL MM1 DO
                                                                                                                                                                                         F(N.X.YP.FH[INDX.*])
                                                                                                                                                                                                                                                                                                                                                                                                                                                                  z
                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                        z
                                                                                                                                                                                                                                                                                                                                                                                                                                                                 1 UNTIL
                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                       STEP 1 UNTIL
                                                                                                                                                 GO TO CORRECT
                                                                                                                                                                                                                                                                        F(N)X)YC)FH[INDX)*1)3
                                                                                                                                                                                                                                                                                                                                                                                                              H(CYI HK)MOD TOP1
                                                                                                                                                                                                                                                                                                                                                                                                                          I=(I3 +K)MDD TQP1
                                                                                                                                                                                                                                                                                                                             11 :=(CYI -M)MDD TQP1
                                                                                                                      GO TO L5
                                                                                                                                                                                                                                                                                                                                                                                                                                                    PFLAG :=TRUE
                                                                                                                                                                                                                                                                                                                                                                                                                                       =MCOEFF[K];
                                                                                                                                                                                                                                                                                                                                                                                                                                                                J := 1 STEP
                                                                                                                                                                                                                                                                                     PFLAG : #FALSE
                                                                                             BEGIN
                                                                                                                                     END ;
                                                                                                                                                                                                                                                                                                                                            T1 SEMCOEFFEM35
                                                                                                                                                                                                                                                                                                                                                         FOR J := 1 STEP
                                                                                                                                                                                                                                 GO TO L2
                                         BEGIN
                                                                                                                                                                                                                                                                                                                                                                                                                                                                                           IF OFLAG THEN
                                                                                                                                                                                                                                                                                                                                                                       IS t≡CYI =0 }
                                                                                                                                                               END
                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                         #
                                                                                                                                                                            END 3
                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                      FOR J
                                                                                                                                                                                                                                             END
                                                                                                                                                                                                                                                          END 3
                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                   JTHEN
                                                                                                                                                                                                                                                                                                                                                                                                                                                                 FOR
                                                                                                                                                                                                                                                                                                  121
                                                                                                                                                                                                                                                                                                                                                                                                BEGIN
                                                                                                                                                                                                                                                                                                                                                                                                                                                                                END ;
```

```
BEGIN
                                                                         00160000
    IF T2 >ERVD[J] × ABS(T3)THEN
                                                                         00161000
    BEGIN
                                                                         00162000
      IF T2 >EAV[J]THEN
                                                                         00163000
      BEGIN
                                                                         00164000
        IF T2 >ERV[J] × ABS(T3)THEN GO TO L4
                                                                         00165000
      END 3
                                                                         00166000
      GD TO L3
                                                                         00167000
    END
                                                                         00168000
  END 3
                                                                         00169000
  C2 1=C2 =M 3
                                                                         00170000
  C2 = C2 / 2.0 
                                                                         00171000
  IF PFLAG THEN FOR J :=1 STEP 1 UNTIL N DO Y[J]:=YP[J]ELSE FOR J :=1 00172000
                                                                         00173000
  STEP 1 UNTIL N DO Y[J]:=YC[J];
  C1 = C1 DIV 2 3
                                                                         00174000
  IF C2 <M THEN GO TO CLOSER J
                                                                         00175000
  INDX 8=INDX +1 ;
                                                                         00176000
  FOR K := 1 STEP 1 UNTIL Q DO
                                                                         00177000
  REGIN
                                                                         00178000
    INDX :=(INDX +1)MOD TQP1 }
                                                                         00179000
    I1 :=(INDX +K)MOD TOP1 ;
                                                                         00180000
    FOR J := 1 STEP 1 UNTIL N DO FH(INDX,J) &= FH(I1,J)
                                                                         00181000
  END J
                                                                         00182000
  GO TO DOUBLER
                                                                         00183000
END 3
                                                                         00184000
J :=0 ;
                                                                         00185000
L3:FOR J := J +1 STEP 1 UNTIL N DO IF (T2 := ABS((T3 := Y[J]) = YM(J]))> EAVOO186000
IJITHEN
                                                                         00187000
BEGIN
                                                                         00188000
  IF T2 >ERV[J]×ABS(T3)THEN
                                                                         00189000
  BEGIN
                                                                         00190000
    L4:INDX :=(CYI =M)MOD TQP1 ;
                                                                         00191000
    00192000
    X :=XF ~C2 ×H ;
                                                                         00193000
    C2 8=C2 +C2 3
                                                                         00194000
    GO TO STARTER
                                                                         00195000
  END
                                                                         00196000
FND J
                                                                         00197000
                                                                         00198000
C2 8=C2 =M 3
IF C2 ≥M THEN
                                                                         00199000
```

BEGINS	00000200
<u>.</u>	00201000
BEGIN	00202000
YMID1[J]:=Y[J];	00203000
=YP[J]}	00204000
MID[J]: HHDM1F[J]	0020200
D ELSE FOR J := 1 STEP	00090200
	0020200
MID1[J] ##Y[J]#	00208000
:YC[J]}	0020300
11FMID[J]:=HDM1F[J]	00210000
	00211000
LAG :=TRUE ;	00212000
CEPT	00213000
n ON	00214000
F PFLAG THEN FOR J 1=1 ST	00215000
IL N DO YEJJ:#YC	00216000
LOSERIIF C2 >0 THEN SHANK	• ER00217000
C1)}	00218000
	00219000
C Q Z	00220000

•					
	•				
		•			
•					
			·	•	
				•	

#### D. The Runge-Kutta-Shanks Method

#### 1. Introduction

The procedure described is a generalization of the Runge-Kutta method for solving a system of differential equations. It may be applied to an arbitrary system of first-order differential equations of the form

$$\vec{y}' = \vec{f} (x, \vec{y})$$

with the initial conditions

$$\vec{y}$$
  $(x_0) = \vec{y}_0$ 

where 
$$\vec{y}(x) = \begin{pmatrix} y_1(x) \\ \vdots \\ y_n(x) \end{pmatrix}$$
, 
$$\vec{y}'(x) = \begin{pmatrix} y_1'(x) \\ \vdots \\ y_n'(x) \end{pmatrix}$$
,

$$\vec{f} (x, \vec{y}) = \begin{pmatrix} f_1 (x, y_1, \dots, y_n) \\ \vdots \\ f_n (x, y_1, \dots, y_n) \end{pmatrix}, \qquad \vec{y}_0 = \begin{pmatrix} y_{10} \\ \vdots \\ \dot{y}_{n0} \end{pmatrix}.$$

#### 2. Description of the Method

The Shanks Method is a single-step procedure for finding a numerical solution of a first-order ordinary differential equation or system of differential equations in which the derivatives of the dependent variables may be expressed explicitly as functions of the independent and dependent variables.

Consider the system of differential equation

$$\vec{y}' = \vec{f}(x, \vec{y})$$
.

Suppose the value of  $\vec{y}$  (x) is known. The value  $\vec{y}$  (x + h) is approximated by

$$\vec{y}$$
 (x + h) =  $\vec{y}$  (x) + h  $\stackrel{m}{\Sigma}$   $\gamma_i$   $\vec{f}_i$  (x,h, $\vec{y}$ ),

where

$$\vec{f}_{1}(x,h,\vec{y}) = \vec{f}(x,\vec{y}),$$

$$\vec{f}_{1}(x,h,\vec{y}) = \vec{f}(x + \alpha_{i}h, \vec{y} + h\sum_{j=1}^{i-1} \beta_{ij}\vec{f}_{j}), i = 2, ..., m.$$

The coefficients  $\alpha_i$  (i = 2, . . ., m),

$$\beta_{ij}$$
 (i = 2, . . ., m; j =1, . . ., i-1), and  $\gamma_i$  (i = 1, . . ., m)

are chosen so as to make the approximation correct to some order. A special case of the Shanks formula is the fourth-order Runge-Kutta formula:

$$\alpha_2 = 1/2$$
,  $\alpha_3 = 1/2$ ,  $\alpha_4 = 1$ ,  $\beta_{21} = 1/2$ ,  $\beta_{31} = 0$ ,  $\beta_{32} = 1/2$ ,  $\beta_{41} = \beta_{42} = 0$ ,  $\beta_{43} = 1$ ,  $\beta_{13} = 1/2$ ,  $\beta_{14} = 1/2$ ,  $\beta_{1$ 

For useful values of the various combinations of  $\alpha$ ,  $\beta$ , and  $\gamma$ , see Shanks [17].

### 3. The Computer Procedure

The procedure was programmed for the B-5500 computer in the B-5500 Algol language. Single precision arithmetic (11 to 12 decimal digits) was used.

## 3.1 Error Estimates and Step Size Control

In this procedure a single set of Shanks formulas is used. Suppose

a vector  $\overrightarrow{y}$  (x) is known. Then the Shanks method is applied to one step of size h(where  $h = \frac{\Delta x}{c}$ ,  $\Delta x$  is the length of the interval, and c is a power of two), and to two steps of size  $\frac{h}{c}$ , as follows:

$$\vec{y}_{p} = \vec{y}(x) + h \sum_{i=1}^{m} \gamma_{i} \vec{f}_{i}(x,h,\vec{y}),$$

$$\vec{y}_{m} = \vec{y}(x) + \frac{h}{2} \sum_{i=1}^{m} \gamma_{i} \vec{f}_{i}(x,h,\vec{y}),$$

$$\vec{y}_{c} = \vec{y}_{m} + \frac{h}{2} \sum_{i=1}^{m} \gamma_{i} \vec{f}_{i}(x + \frac{h}{2}, \frac{h}{2}, \vec{y}_{m}).$$

Both  $\vec{y}_p$  and  $\vec{y}_c$  are estimates of  $\vec{y}(x+h)$ . An error estimate  $E_k = \frac{|\vec{y}_{ck} - \vec{y}_{pk}|}{f}$  (where f is an empirical factor) is calculated for each independent variable  $y_k$ . If both  $E_k > \frac{E_{ak}}{c^p}$  and  $E_k > \frac{E_{rk}|\vec{y}_{ck}|}{c^p}$  for any dependent variable where  $E_{ak}$  is an absolute error estimate,  $E_{rk}$  is a relative error estimate, and p is an input parameter, usually 1 or 1/2, then the step is rejected and the step size is halved; otherwise the step is accepted and  $\vec{y}_c$  is taken as the vector  $\vec{y}(x+h)$ . If for every dependent variable, either  $E_k > \frac{E_{ak}}{2(j+3)}$  or  $E_k > \frac{E_{rk}|\vec{y}_{ck}|}{2(j+3)}$ , where j is the order, then the step size is doubled. If the step size h is larger than the distance to the end of the interval, then that distance is taken as the step size.

### 3.2 Input and Output of the Procedure

The procedure is called as follows:

SHANKS (N,XI,XF,YV,F,M,ORDER,CF,P,EA,ER,DX);

where the parameters have the following meaning:

N - number of dependent variables;

XI - initial value of the independent variable;

XF - final value of the independent variable;

- YV array of initial values of the dependent variables, based at zero but with the zero element not used;
- F a function evaluation procedure, supplied by the user, called as follows  $F({\tt N},{\tt X},{\tt YV},{\tt FV});$

where N is the number of dependent variables, X is the value of the independent variable, YV is the array of values of the dependent variables, and FV is the array in which the function values are placed;

M - the number of function evaluations in each application of the Shanks method;

ORDER - the order of the Shanks formulas used;

- CF the array of Shanks coefficients, starting in the zero element arranged as follows: for each i, the corresponding  $\alpha_i \beta_{ij}$ 's, followed by  $\alpha_i$ , with the  $\gamma_i$ 's at the end;
- P an exponent (usually 1/2 or 1) used in step size control (1 assuming the errors are additive; 1/2 assuming that they are random);
- EA an array of absolute error asked;
- ER an array of relative error asked;
- DX a recommended starting step size (the actual starting step size will be  $\frac{XF XI}{c}$ , where c is the smallest power of 2 for which  $\left|\frac{XF XI}{c}\right| \le \left|\frac{DX}{c}\right|$ ).

The final values of the dependent variable are stored in YV before exiting the procedure.

# 4. Flow Diagram and Program Listing

Figure 4 is the flow diagram for the Runge-Kutta-Shanks procedure.

A listing of the program is given at the end of this section.

## 5. Results and Conclusions

This procedure was used with systems of differential equations with

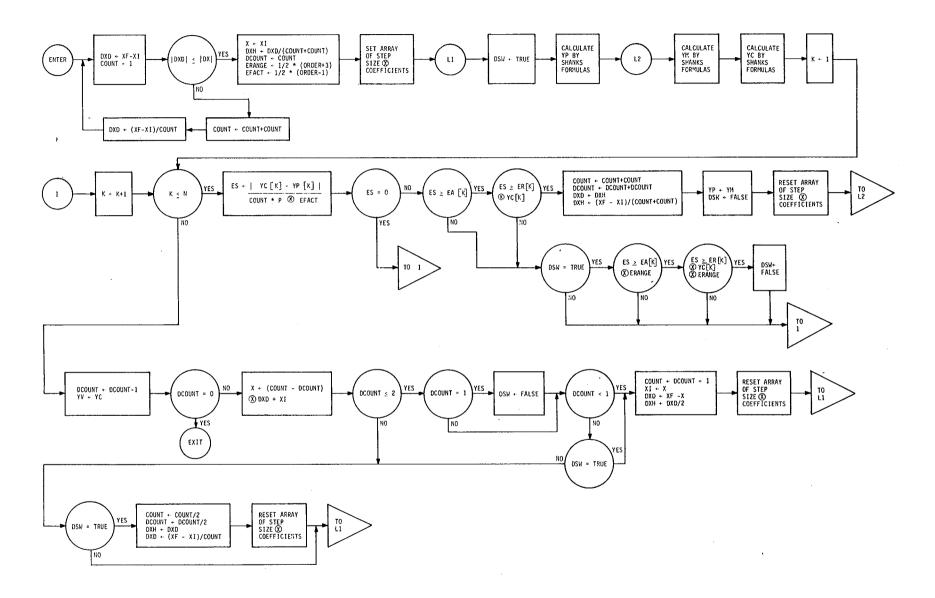


Figure 4. Flow Diagram for the Runge-Kutta-Shanks Procedure.

analytic solutions, as well as with the three-body problem. It gave slightly more accuracy than was asked.

In order to reach the end of the interval more accurately, the steps taken were binary fractions of the total interval. Hence, it was necessary to use halving and doubling rather than the continuous step size control of previous experiments [18]. Although this caused the rejection of more steps, it prevented roundoff in the independent variable.

The procedure was first run without the empirical factor f (i.e., with f=1) mentioned in 3.1. The results were more accurate than asked.

The theoretical value,  $f = \frac{1}{2^{\text{order}}-1}$ , was then used. It was found that for some formulas (in particular, 8-10 and 8-12), the desired accuracy was not reached.

Finally, runs were made with a compromise value,  $f = \frac{1}{2}$  order-1. In this case, the results were good for most formulas, but the Shanks 8-10 formulas still sometimes did not obtain the desired accuracy.

It might be noted that the most accurate results were usually obtained with the Shanks 4-4 formulas.

It is recommended that further experimentation be done in the area of step-size control with the Runge-Kutta-Shanks method. In particular, other values for the factor f might be used. It might be desirable to determine a particular constant for each set of formulas.

```
Š
```

00066000	NCLI+(W×W+W)DIA S+W+W}
0008£000	DKIB+03
0007£000	EFACTUR+COUNT*P×EFACT;
00098000	EFACT+4/EFACT3
0003£000	ERANGE+0.125/EFACT;
00076000	FOR I+1STEP 1UNTIL ORDER DO EFACT+EFACT;
00055000	EFACT + 13
00035000	DCONNI+CONNI)
00031000	DXH+DX1\CONNIS;
00030000	COUNT2+COUNT+COUNT;
00050000	END)
00088000	
00072000	DXD+DX1\CDNN1}
00056000	CDUNT+CDUNT+CDUNT3
00052000	BECIN
00024000	MHIFE ABS(DX) <abs(dxd)do< td=""></abs(dxd)do<>
00053000	COUNT+13
00055000	IE DX⇔ÒTHEN DX←DXD3
00021000	IF DXT=OTHEN GO TO EXITS
00050000	DXD+DXI+XF-XIJ
00061000	\$1EP\$+\$1EPR+0\$
00081000	fI=W→W
00071000	INTEGER STEPR, STEPS;
00091000	LABEL L1, L2, EXIT
000\$1000	DEFINE CFH≖CFD#3
00011000	REAL ARRAY CFD[0:(M+3)×M-2] FV[0:M-1.0:N].GV.YC.YM.YP[0:N];
00013000	BOOFEVN CESM.DSW.
00015000	REAL BETA, DCOUNT, DXD, DXH, DXT, EFACTOR, ERANGE, ES, GAMMA, X, XM;
00011000	REAL EFACT!
0001000	INTEGER OKTRJ
00060000	INTEGER NOF13
00080000	INTEGER I.J.K.L.COUNT.COUNTZ.II.NCFJ
00020000	BECIN
00090000	
0000000	PROCEDURE F3
00000000	REAL ARRAY YV.CF.EA.ER[0];
00005000	BEVT XI'XL'b'DX)
0002000	INTEGER Now ORDERS
00000000	AAFUE WAXIAXFAMAUROERAPANA
	PROCEDURE SHANKS(N.XI.XF.YV.F.M.ORDER.CF.P.F.ER.ER.DX);

```
00040000
NCF + NCF 1 + 1;
CFSW+FALSEJ
                                                                         00041000
FOR I+OSTEP 1UNTIL NCF1 DO
                                                                         00042000
REGIN
                                                                          00043000
                                                                          00044000
  CFD[I]+CF[I]×DXD3
                                                                          00045000
  CFH[I+NCF]+CF[I1×DXH3
                                                                          00046000
                                                                          00047000
END!
X+XI3
                                                                          00048000
                                                                          00049000
KHXO+IX+MX
                                                                          00050000
L1:DSW+TRUE;
                                                                          00051000
F(No Xo YVo GV)
                                                                          00052000
IF CFSW THEN L+NCF1 ELSE L+=13
FOR I+1STEP 1UNTIL M DO
                                                                          00053000
                                                                          00054000
BEGIN
                                                                          00055000
  II+I-13
                                                                          00056000
  L+L+13
  BETA+CFD[L];
                                                                          00057000
  FOR K41STEP 1UNTIL N DO YP[K]+GV[K]*BETA+YV[K];
                                                                          00058000
  FOR J41STEP 1UNTIL II DO
                                                                          00059000
                                                                          00060000
  BEGIN
                                                                          00061000
    L+L+13
                                                                          00062000
    BETA+CFD[L];
    FOR K+1STEP 1UNTIL N DO YP[K]+FV[J,K]*BETA+YP[K]}
                                                                          00063000
                                                                          00064000
                                                                          00065000
  END)
                                                                          00066000
  L+L+13
                                                                          00067000
  F(N,CFD[L]+X,YP,FV(I,*1))
                                                                          00068000
                                                                          00069000
END3
                                                                          00070000
L+L+13
                                                                          00071000
GAMMA+CFDrL33
FOR K+1STEP 1UNTIL N DO YPEK1+GVEK1×GAMMA+YVEK13
                                                                          00072000
FOR I + 1 STEP 1UNTIL M DO
                                                                          00073000
                                                                          00074000
BEGIN :
                                                                          00075000
  L+L+18
                                                                          00076000
  GAMMA&CFD[L]3
  FOR K41STEP 1UNTIL N DO YPEKJ&FVEI&KJ×GAMMA+YPEKJ;
                                                                          00077000
                                                                          00078000
                                                                          00079000
END3
```

```
L2: IF CFSW THEN L+=13
                                                                       00080000
FOR I+1STEP 1UNTIL M DO
                                                                       00081000
BEGIN
                                                                       00082000
  II+I-13
                                                                       00083000
  L+L+13
                                                                       00084000
  BETA+CFH[L];
                                                                       00085000
  FOR K+1STEP 1UNTIL N DO YMEK1+GVEK1×BETA+YVEK1;
                                                                       00086000
  FOR J+1STEP 1UNTIL IT DO
                                                                       00087000
  BEGIN
                                                                       00088000
    L+L+13
                                                                       00089000
    BETA+CFHEL];
                                                                       00090000
    FOR K+1STEP 1UNTIL N DO YM(K)+FV(J,K)×BETA+YM(K);
                                                                       00091000
                                                                       00092000
  ENDI
                                                                       00093000
  L+L+13
                                                                       00094000
  F(N,CFH[L]+X,YM,FV[I,*]);
                                                                       00095000
                                                                       00096000
END;
                                                                       00097000
L+L+13
                                                                       00098000
GAMMA+CFH[L];
                                                                       00099000
FOR K+1STEP 1UNTIL N DO YM[K]+GV[K]×GAMMA+YV[K];
                                                                       00100000
FOR I+1STEP 1UNTIL M DO
                                                                       00101000
BEGIN
                                                                       00102000
  L+L+13
                                                                       00103000
  GAMMA+CFH[L];
                                                                       00104000
  FOR K+1STEP 1UNTIL N DO YM(K)+FV(I)KJ×GAMMA+YM(K);
                                                                       00105000
                                                                       00106000
END!
                                                                       00107000
F(N,XM,YM,FV[O,*]);
                                                                       00108000
IF CFSW THEN L+=1ELSE L+NCF13
                                                                       00109000
FOR I+1STEP 1UNTIL M DO
                                                                       00110000
BEGIN
                                                                       00111000
  II+I=13
                                                                       00112000
  FOR K+1STEP 1UNTIL N DO YC[K]+YM[K];
                                                                       00113000
  FOR J+OSTEP 1UNTIL II DO
                                                                       00114000
  BEGIN
                                                                       00115000
    L+L+13
                                                                       00116000
    BETA+CFH[L];
                                                                       00117000
    FOR K+1STEP 1UNTIL N DO YCIKJ+FV(J,K)×BETA+YC(K);
                                                                       00118000
                                                                       00119000
```

```
00120000
  FND;
                                                                         00121000
  L+L+13
                                                                         00122000
  F(N,CFH[L]+XM,YC,FV[I,*]);
                                                                         00123000
                                                                         00124000
END!
                                                                         00125000
FOR K+1STEP 1UNTIL N DO YC(K)+YM(K);
                                                                         00126000
FOR I+OSTEP 1UNTIL M DO
                                                                         00127000
REGIN
                                                                         00128000
  L4L+13
                                                                         00129000
  GAMMA+CFHEL];
                                                                         00130000
  FOR K41STEP 1UNTIL N DO YCCKJ+FVCI>KJ×GAMMA+YCCKJ;
                                                                         00131000
                                                                         00132000
END!
                                                                         00133000
FOR K+1STEP 1UNTIL N DO
                                                                         00134000
BEGIN
                                                                         00135000
  ES+ABS(YC[K]=YP[K]) XEFACTOR;
                                                                         00136000
  IF ES≠OTHEN
                                                                         00137000
  REGIN
  IF ES≥EA[K]THEN IF ES≥ABS(YC[K])×ER[K]THEN
                                                                         00138000
                                                                         00139000
    BEGIN
                                                                         00140000
      DSW+FALSE3
                                                                         00141000
      STEPR+STEPR+13
                                                                         00142000
      COUNT+COUNT2;
                                                                         00143000
      COUNT2+COUNT+COUNT)
                                                                         00144000
      DCOUNT+DCOUNT+DCOUNT;
                                                                         00145000
       DXD+DXH3
                                                                         00146000
      DXH+DXT/COUNT23
                                                                         00147000
       FFACTOR+COUNT*PXEFACT;
                                                                          00148000
      IF CFSW THEN
                                                                         00149000
       BEGIN
         FOR 1+OSTEP 1UNTIL NCF1 DO CFH[I+NCF]+CF[I]×DXH;
                                                                          00150000
                                                                          00151000
         CFSW+FALSE)
                                                                          00152000
                                                                          00153000
       END ELSE
                                                                          00154000
       BEGIN
                                                                          00155000
         FOR I+OSTEP 1UNTIL NCF1 DO CFH[]+CF[]*DXH;
                                                                          00156000
         CFSW+TRUE;
                                                                          00157000
                                                                          00158000
       END)
                                                                          00159000
       XM+(COUNT2+1-DCOUNT-DCOUNT) XDXH+XI;
```

OR KAISTEP IUNTIL N DO YPPKIAYMEKI;	016000
	016200
THEN I	00163000
)SW+FALSE!	016500
	016600
	016700
	016800
€ CN	016900
COUNT+DCOUNT+13	017000
	017100
00	017200
EXIT	017300
<b>-</b>	017400
EGIN	017600
IF OCCUNTEITHEN DSW-FALSE;	017700
뽀	017800
1	017900
ASSESSED TO THE TRANSPORT OF THE TRANSPO	018000
COUNTACTOR OF	018100
COUNTS+2>	018200
CHACTORATE ACTOR	018300
	018400
	018500
13/0/0/53 13/0/12/23	018600
	018700
	018800
STATE TONIL NOTE DO	018900
2	019000
0.3	019100
	019200
	019300
	019400
	019500
	019600
	019700
	019800
	019900

IF DSW THEN	0030000
BEGIN	00201000
DKTR+DKTR+13	00202000
COUNT2+COUNT3	00203000
COUNT+COUNT DIV 2;	00204000
DCOUNT+DCOUNT/2;	00205000
DXH+DXD3	00206000
DXD+DXT/COUNT;	00207000
EFACTOR+COUNT*P×EFACT;	00208000
IF CFSW THEN	00209000
BEGIN	00210000
FOR I+OSTEP 1UNTIL NCF1 DO CFD[I]+CF[I]×DXD}	00211000
CFSW+FALSE)	00212000
	00213000
END ELSE	00214000
BEGIN	00215000
FOR I+OSTEP 1UNTIL NCF1 DO CFD[I+NCF]+CF[I]×DXD}	00216000
CFSW+TRUE;	00217000
	00218000
END)	00219000
	00220000
END;	00221000
<pre>XM &lt; (COUNT2+1 = DCOUNT = DCOUNT) × DXH + XI;</pre>	00555000
GO TO L1;	00223000
EXIT:	00224000
END;	00225000

.

### E. The General Multistep Method Starting Procedure

#### 1. Introduction

The general multistep method starting procedure is a B-5500 ALGOL single-precision Runge-Kutta-Shanks procedure used for obtaining starting values for the Adams, Butcher, and Cowell multistep methods. The declaration is as follows:

integer procedure start (m, xi, xf, cl, ea, er, f, m, x, yiv, yh, fh, yfv, cyi, cym, pa, p, fneval, rksconst);

value n, xi, xf, cl, m, cyi, cym, per, p, fneval;
integer n, cl, m, cyi, cym, pa, fneval
real xi, xf, x, p;
real array ea, er, yiv, yfv, rksconst [0], yh, fh [0,0];
procedure f;

#### 2. Description of the Procedure

The parameters of the procedure are defined as follows:

- n the number of dependent variables
- $\underline{\mathtt{xi}}$  the starting value of the independent variable x passed to the multistep method
- $\underline{\mathrm{xf}}$  the final value of the independent variable x passed to the multistep method
  - cl the integer counter (xf xi)/h from the multistep method
  - ea the absolute error vector passed to the multistep method
  - $\underline{\mathrm{er}}$  the relative error vector passed to the multistep method
  - $\underline{f}$  the procedure which computes  $\overrightarrow{f}(x, y) = \overrightarrow{y}'$
  - m the number of history points to be calculated by start

- $\underline{x}$  the value of the independent variable at which  $\underline{start}$  begins its integration
- $\underline{yiv}$  the array which contains on entry for Adams and Cowell the values of the dependent variables at  $\underline{x}$  and which contains on exit for Cowell the values of the dependent variable at the mth point calculated by  $\underline{start}$
- $\underline{yh}$  the array which contains on entry for Butcher in row  $\underline{cyi}$  the values of the dependent variables at  $\underline{x}$  and which contains on exit for Butcher the values of the dependent variables at each of the m points calculated by  $\underline{start}$
- $\underline{\underline{fh}}$  the array which contains on entry in row  $\underline{\underline{cyi}}$  the function values at  $\underline{\underline{x}}$  and which contains on exit the function values at each of the m points calculated by start
- y f v the array which contains on exit the values of the dependent variables at the mth point calculated by start for Adams or the m/2th point calculated by start for Cowell
- $\underline{cyi}$  the cyclic index identifying on entry the row of  $\underline{yh}$  in which the values of the dependent variables at  $\underline{x}$  are stored for Butcher and the row of  $\underline{fh}$  in which the function values at  $\underline{x}$  are stored for any method
  - cym the number of rows in the arrays yh and fh
  - pa the parameter which is zero for Adams, one for Cowell, two for Butcher
- $\underline{p}$  the exponent such that the absolute error at each step is not to exceed  $\underline{ea/cl}^{\underline{p}}$  and the relative error at each step is not to exceed  $\underline{er/cl}^{\underline{p}}$
- <u>fneval</u> the number of function evaluations required by the Runge-Kutta-Shanks procedure

 $\underline{\text{rksconst}}$  - the array which contains the Runge-Kutta-Shanks coefficients in the same order as required by the procedure  $\underline{\text{shanks}}$  described in section  $\underline{\text{D}}$ .

The value of  $\underline{\text{start}}$  on exit is two to the power of the number of halvings which took place within start.

Although the base of the arrays <u>ea</u>, <u>er</u>, <u>yiv</u>, and <u>yfv</u> and of the rows of <u>yh</u> and <u>fh</u> is zero, the n components are placed in position 1, 2, ..., n and the zero position is unused.

The procedure attempts to calculate m (if m is even and positive) or m+1 (if m is odd) Runge-Kutta-Shanks steps of size h=(xf-xi)/cl. After each even step of size h is taken, one step of size 2h is taken over the interval spanned by the two steps of size h. The absolute value of the differences in each dependent variable between the 2h-step and the second h-step is compared with the corresponding component of  $\vec{ea}/(cl/2)^p$  for absolute error and with the product of the corresponding component of  $\vec{er}/(cl/2)^p$  and the corresponding dependent variable value from the second h-step for relative error. If each component of the difference does not exceed in either the absolute or the relative error test and m steps have not yet been taken, the process of two h-steps, one 2h-step, and test is continued. If any component of the difference exceeds in both the absolute and the relative error tests, cl is doubled, h is halved, and integration begins again at x. The first step of previous size h was saved and becomes the first step of present size 2h.

The m calculated function values from h-steps are placed in rows (cyi+1) mod cym, (cyi+2) mod cym, ..., (cyi+m) mod cym of the array fh. For Butcher, the corresponding dependent variable values from h-steps are placed in the corresponding rows of the array yh; if m is odd, the values of the dependent

variable after h-step m + l are placed in row (cyi + m + l) mod cym of yh. For Adams, the dependent variable values from h-step m are placed in the array yfv. For Cowell, the dependent variable values from h-step m are placed in the array yiv and from h-step m/2 (m is always even for Cowell) are placed in yfv. If m is zero, no calculation takes place.

### 3. Flow Diagram and Program Listing

Figure 5 is the flow diagram for the starting procedure. The program listing follows at the end of this section.

	The second secon	to white the control of the control	المرواقي والهواز ويند والمعاهدة كالمحاطفة والمعادية	til sammanna sammanni siyati samsan	والماد المعالمة المعا	والأي السيطية والأراب فالماكاتين	
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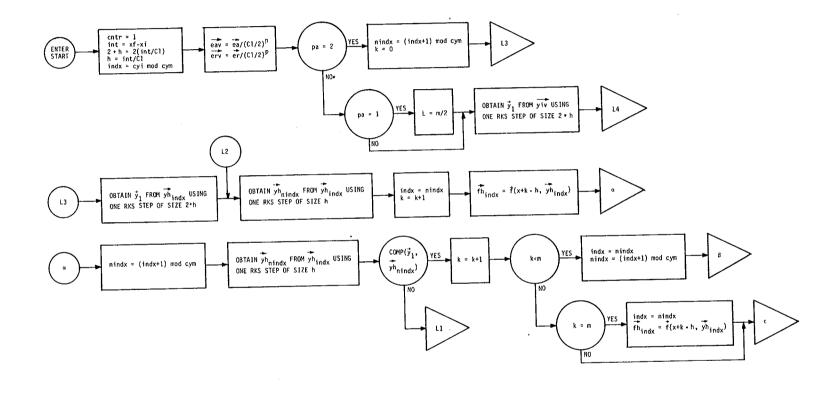


Figure 5. Flow Diagram for the General Multistep Method Starting Procedure.

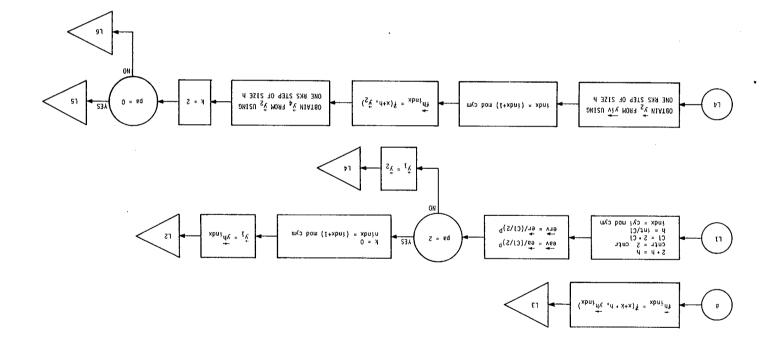


Figure 5 (Continued). Flow Diagram for the General Multistep Method Starting Procedure.

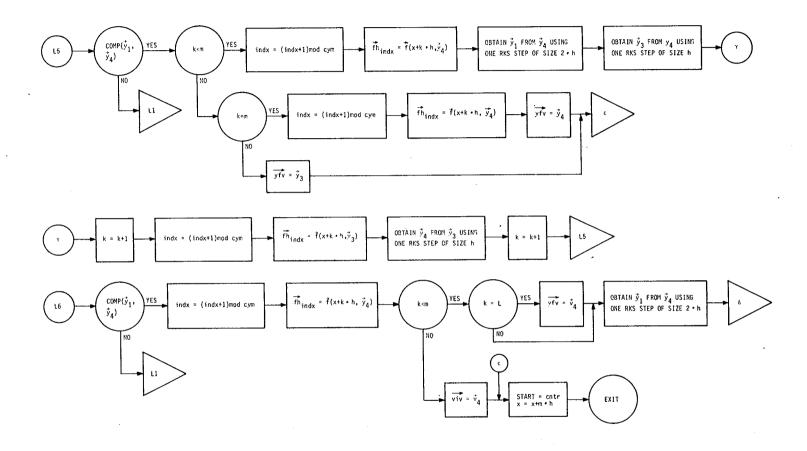


Figure 5 (Continued). Flow Diagram for the General Multistep Method Starting Procedure.

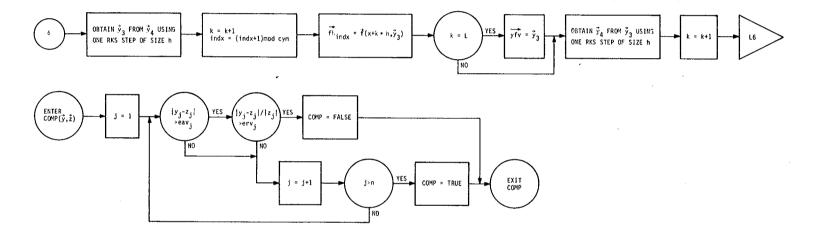


Figure 5 (Continued). Flow Diagram for the General Multistep Method Starting Procedure.

```
LEMP :=CDEFF[CCNT 8=CCNT +133
00066000
                                                                         BECIN
00086000
                                              FOR K := 0 SIEP 1 UNTIL FUMAX DO
00035000
                     FOR J := 1 SIEP 1 UNTIL N DO YFV[J]:=FV[J]XTEMP +YIV[J]
00036000
                                                                         END 1
00032000
                                               LEMP : #COEFF[CCMT : #CCMT +1]
00034000
                                  E(N'X +CDEEECCONT *=CCNT +11 > XEA + CTI+1))
00055000
                                                                       END 1
00032000
                 FOR J := 1 SIEP 1 UNTIL N DO YFV[J] := G[K.J] xTEMP +YFV[J]
00031000
                                            LEMb := COELL[CCN1 := CCN1 +1])
00006000
                                                                       BECIN
00053000
                                             LOB K 1=0 21Eb 1 ONLIF I =1 DO
00088000
                    FOR J ##1 STEP 1 UNTIL N DO YFVLJJ##FVLJJ×TEMP +YIV[J]
00022000
                                                                         BECIN
00052000
                                              FOR I :=0 SIEP 1 UNTIL FUMAX DO
00022000
                                                       LEMB :=CUELL[CCNI :=0]}
00054000
                                                                   REAL TEMP &
00023000
                                                          INTEGER INDOKACONT A
00022000
                                                                           BECIN
00051000
00050000
                                                                   PROCEDURE F 3
00061000
                                         REAL ARRAY COEFF, YIV, YFV, FV[0], G[0,0].
00081000
                                                                         REAL X 3
00011000
                                                               INTEGER N'FUMAX 3
00091000
                                                               VALUE NAXAFUMAX &
00051000
                              PROCEDURE RUNKUT(N.X.FUMAX.COEFF.YIV.YFV.FV.F.G.)
00011000
                                                       00013000
                                                         *MI*CLO:FNEVAL -2.0:NJ$
00011000
REAL ARRAY HC.TWOHCLO:((FUEVAL+3)×FUEVAL)/20-23.EAV.FRVFY12Y2.Y3.Y4C000011000
                                                            REAL INTAHOTMOHATE &
00001000
                               INTEGER IS IN TACOUNTERMANT INDX NINDX COLR 3
00060000
                                                                              BECIN
00080000
00020000
                                                                      PROCEDURE F 3
00090000
                                 REAL ARRAY EASER, YIV, YFV, RKSCONST[0], YH, FH[0,0]!
00050000
                                                                   REAL XI,XF,X,P J
000040000
                                                INTEGER WICTIMICYINCYMIPAFREVAL 3
00003000
                                          VALUE N.XI.XF. CI.M.CYI.CYM.PAPPFREVAL F
00005000
                                                               * b * ENEVAL * RKSCOUST) }
00010000
INTEGER PROCEDURE START(NAXIAXFACIAEA ERAFAMAXATIVAYHAFHAYFVACYIACYMAPA 00000000
```

TO A STANCE OF THE STANCE OF THE SECOND SECTION OF THE SECOND SEC

```
FOR J := 1 STEP 1 UNTIL N DO YFV[J]:=G[K,J]xTEMP +YFV[J]
                                                                         00040000
 END 3
                                                                         00041000
                                                                         00042000
FND J
                                                                          00043000
BOOLEAN PROCEDURE COMP(N, EAV, ERV, Y, Z);
                                                                          00044000
VALUE N J
                                                                          00045000
INTEGER N J
                                                                         00046000
REAL ARRAY EAV, ERV, Y, Z[0];
                                                                         00047000
                                                                         00048000
BEGIN
                                                                         00049000
  INTEGER J 3
                                                                         00050000
 REAL T1 3
                                                                         00051000
 LABEL L1 3
                                                                         00052000
 FOR J == 1 STEP 1 UNTIL N DO IF (T1 == ABS(Y[J]=Z[J]))>EAV[J]THEN
                                                                         00053000
 BEGIN
                                                                         00054000
    IF T1 >ERV[J] × ABS(Z[J]) THEN
                                                                         00055000
    BEGIN
                                                                         00056000
      COMP :=FALSE ;
                                                                         00057000
      GO TO L1
                                                                         00058000
    END
                                                                         00059000
 END 3
                                                                         00060000
 COMP :=TRUE ;
                                                                         00061000
 L1:
                                                                         00062000
END 3
                                                                         00063000
CNTR ##1 3
                                                                         00064000
IF M ≠0 THEN
                                                                         00065000
BEGIN
                                                                         00066000
 COEFFCNT ==(((FNEVAL +3)×FNEVAL)/2)=2 }
                                                                         00067000
 FNMAX I=FNEVAL =2 3
                                                                         00068000
 INT :=XF =XI ;
                                                                         00069000
 TWOH :=(INT +INT)/C1 ;
                                                                         00070000
 H #= INT /C1 3
                                                                         00071000
 FOR I == 0 STEP 1 UNTIL COEFFCNT DO
                                                                         00072000
 BEGIN
                                                                         00073000
   HC[];=(T1 ;=RKSCONST[])×H;
                                                                         00074000
    TWOHC[I]:=T1 xTWOH
                                                                         00075000
 END 3
                                                                         00076000
 INDX : #CYI MOD CYM ;
                                                                         00077000
 T1 ##(C1 /2)*P #
                                                                         00078000
 FOR J := 1 STEP 1 UNTIL N DO
                                                                         00079000
```

```
98
```

```
00061100
                                         E(NOK XH +XDAH[INDXD*]DEH[INDXD*])}
00081100
                                                   MINDX 8=(INDX +1)WOD CAW }
00011100
                                                                f XONIN=: XONI
00091100
                                                                    f I+ N=1 N
00051100
                                                                             11
ΓS:kNNKN1(N⊅K ×H +X⊅ENW∀X⊅HC⊅AH[INDX⊅*]⊅AH[NINDX⊅*]⊅EH[INDX⊅*]⊅E→@00117000
0001100
                                                                         END ?
00115000
                                                         Y1[J] = TH[NINDX D]
00011100
                                                         ERV[J]:=ER[J]/RI J
00001100
                                                         EAVEU31=EELU3VA1 3
00060100
                                                                         BECIN
                                                 FOR J := 1 SIEP 1 UNTIL N DO
00080100
00070100
                                                   MINDX == CINDX +1)WOD CAW }
00090100
                                                                       K == 0 }
00050100
                                                                           BECIN
00010100
                                                                   IL by =5 THEN
000103000
                                                                11 :=(C1 \S) +b }
00102000
                                                           INDX #=CAI WOD CAW }
00010100
                                                                           END )
00000100
                                                         HC[I]: #BK2CON21[I]×H
00066000
                                                              IMOHC[1]:=HC[1])
00086000
                                                                           BECIN
                                            FOR I := 0 SIEP I UNTIL COEFFCNT DO
00026000
00096000
                                                                   H STINI VCI }
00056000
                                                                   f 10+ 10=: 10
00006000
                                                             CNIK S = CNIK + CNIK 1
00088000
                                                                   1 H=: HOMI:IT
00035000
                                                                      6 10 LO E4 3
                                RUNKUT(NoxoFNMAXoTWOHCoYIVoY1oFHCINDXo+loFog) #
00016000
00006000
                                                    IL BY #1 THEN F 3=W DIA S }
00068000
                                                                            END 1
00088000
                                                                      60 TO L3
00078000
                                                                       K 1 = 0 }
00098000
                                                   NINDX :=(INDX +1)WOD CAW }
00088000
                                                                           BECIN
00084000
                                                                   IE BY #5 THEN
00088000
                                                                            END 1
00088000
                                                              ERVIU1:=ERIU1/T1
                                                           EAVIJ1=EAIJVAJ
00018000
00008000
                                                                           BECIN
```

```
00065100
                  RUNKUICU.K XH +X, FUMAX, TWOHC, Y4, Y1, FH[INDX, + ], F, G);
00085100
                                            ECN'SK XH +X > A T > L I ND X > X ] ) }
00015100
                                              INDX :=(INDX +1)WOD CAW 1
00095100
                                                                      BECIN
00055100
                                                              IE K <W LHEN
00075100
                                                                        BECIN
00025100
                                            FRITE COMP(N)EAV)ERV, YI, Y4) THEN
00125000
                                                                          RECTA
00015100
                                                                  IF PA =0 THEN
00005100
                                                                        K =5 }
                              RUNKUT(N.X +H.FUMAX.HC.Y2.Y4.FH[INDX.*1.F.G.);
0006#100
00084100
                                                      E(N°X +H°AS°EH[INDX°*])}
00027100
                                                     INDX :=(INDX +I)WOD CAW }
0009#100
                              L4:RUNKUT(N,X,FUMAX,HC,YIV,Y2,FH[INDX,*],F,G)J
00057100
                                                                          E ON 3
00011100
                                                                 0001000
                                                          ERV[J]:=ER[J]/T1 ;
00145000
                                                          EAV[J]:=EA[J]/T1 }
0001#100
                                                                          RECIN
00001100
                                                  FOR J := 1 SIEP 1 UNTIL N DO
00068100
                                                                            BECIN
00088100
                                                                         END ETZE
00015100
                                                             END ELSE GO TO L1
00098100
                                                                          END.
00056100
                                      E(N*K xH +X* \ H [ I N D X * ] * E H [ I N D X * ] )
00045100
                                                            f XUNIN=: XUNI
000223000
                                                                        BECIN
00135000
                                                                IL K =W THEN
00012100
                                                                        END 1
00006100
                                                                   GO TO L2
F3:BONKOICN'K XH +X'ENWXX'IMOHC'AHCINDX'*]'AT'EHCINDX'+]'E'C)10015000
00128000
                                     E(N'K XH +X\XH[INDX\*]\EH[INDX\*])}
00127000
                                               NINDX : #(INDX +1)WOD CAW }
00156000
                                                            f XONIN=: XONI
00152000
                                                                        BECIN
00154000
                                                                IL K <W THEN
00153000
                                                                   K :=K + 1 }
00155000
                                                                          BECIN
00121000
                                       IF COMP(N.EAV.ERV.Y1.YH[NINDX.*])THEN
BUNKUTCN.K XH +X.FRMAX.HC.YHEINDX.*1.YHENINDX.*1.FHEINDX.*1.FF.G.); 00120000
```

```
END :
00066100
                                                                 X+ Hx W=: X
00086100
                                                                       END 1
00016100
                                                                       END
00096100
                                                       END EFRE GO TO LI
00056100
                            FOR J := 1 SIEP 1 UNTIL N DO YIV[J] = Y4[J]
00006100
                                                                 END 1
00163000
                                                            97 01 09
00165000
                                                          K 1=K +1 }
00016100
                    RUNKUTCN.K xH +X2FNMAX2HC2Y32Y42FHEINDX2+12F5G)$
00006100
             IE K = T THEN FOR J := 1 STEP 1 UNTIL N DO YFV[J] = Y3[J] }
00069100
                                         E(N'K XH +X'A3'EH[INDX'+])}
00088100
                                           INDX :=(INDX +I)WGD CAW 1
00078100
                                                          K t=K +1 }
00098100
                    RUNKUTCN.K ×H +X.FUMAX.HC.Y4.7.FHEINDX.+1.FF.G.)!
00058100
                 RUNKUTCNøK ×H +XøFNMAXøTWOHCøY4øY1øFHEINDXø*3øFøG)$
00048100
             00028100
                                                                 BECIN
00782000
                                                          IE K <W THEW
00018100
                                           E(Nok xH +XoAdoEH[INDX++])}
00008100
                                             INDX :=(INDX +1)WOD CAW }
00062100
                                                                   BECIN
00087100
                                         TREIL COMB(N'EBADERADATEM
00017100
                                                                     BECIN
00092100
                                                                   END FERF
00051100
                                                       END EFRE CO 10 FT
00011100
                    END ELSE FOR J :=1 STEP 1 UNTIL N DO YFVIJ1=Y3[J]
00057100
                           FOR J := 1 SIEP 1 UNTIL N DO YFV[J] := 44[J]
00115000
                                         E(N'K XH +X'A X + LINDX + 1))
00017100
                                            INDX ==(INDX +I)WOD CAW 1
00007100
                                                                  BECIN
00069100
                                                           IE K =W THEW
00089100
                                                                  END 1
00049100
                                                             90 In F2
00099100
                                                           K 1=K +1 }
00059100
                     RUNKUTCN.K ×H +X.FNMAX.HC.Y3.Y4.FH[INDX.+1.F.G.);
 00019100
                                          E(NºK xH +XºA3ºEH[INDXº#]))
 00029100
                                            INDX # CINDX +1) WOD CAW 1
 00195000
                                                           K 1=K +1 }
 00019100
                     RUNKUT(Nok xH +XoFNMAXoHCoY4oY3oFHLINDXo+ JoFoG);
 00009100
```

START := CNTR ;

END 1

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#### III. THE EXECUTIVE PROCEDURE

#### A. <u>Introduction</u>

The executive procedure acts in an administrative and supervisory capacity. It does the bookkeeping and makes the decisions as to which methods are to be used, but does none of the actual integration. The executive procedure uses as subprocedures five basic integration routines; these are:

- 1) The Adams-Bashforth-Moulton routine,
- 2) The Stetter-Gragg-Butcher routine,
- 3) The Cowell constant Nth order difference routine,
- 4) The Runge-Kutta-Shanks routine,
- 5) The start and restart routine (containing a separate Runge-Kutta-Shanks routine).

These five basic routines do the actual integration. Each is described in Chapter II of this report.

The executive procedure works in the following way. When a call is made in the procedure to integrate from point a to the point b, this interval is divided into eighths. The first eighth of the interval is integrated by one method for each of two different orders, and the time taken by each recorded. The second eighth is integrated by another method, also for two different orders, and the times recorded. The winners then compete against each other over the next fourth of the interval. That is, the fastest order of the first method and the faster order of the second method are both used to integrate the second fourth of the interval, and the time taken by each recorded. The faster method of these two is then presumably the best (fastest) of the four tried, and it is used (alone) to integrate over the last half of the interval.

All of the times measured above are then logged in a cumulative history file and the winners and losers noted.

This file then is used as the basis of selecting which methods and orders are chosen each time. The selection process is as follows: The first of the two methods is chosen at random. The second method is chosen to be the method showing the best history of success among the three remaining methods. Then within each method the same kind of selection process with respect to orders is used. In this way the past performance of the different methods and orders influences the choice of which are allowed to compete, such that the more successful have a higher probability of being selected.

#### B. The Selection Process

There are four methods available for the integration process, and within each method there are four orders available. The methods and orders are as follows:

- 1) The Adams method with orders 4(4), 5(4), 6(4), 7(5).
- 2) The Butcher formulas with orders 3(4), 5(4), 7(4), 7(5).
- 3) The Cowell method with orders 7(5), 9(5), 11(5), 13(5).
- 4) The Shanks formulas with orders 4, 5, 6, 7.

Each order of each multistep method has an associated Runge-Kutta-Shanks restart procedure order given in parenthesis after the method order. Details on these methods are given in Chapter II of this report. The magnetic tape containing the coefficients has several additional orders of each method, but the program is now set to use just those mentioned above.

The selection process is the following. The first of two methods is chosen at random (using a random number generator) from among the four

available. The second method is chosen to be the method showing the best history of success among the three remaining methods, with the cumulative history file being used to determine the degree of success. Then within each method the same kind of selection process with respect to orders is used. That is, the first order is chosen at random, and the second order is chosen on the basis of which of the remaining three has been the most successful (fastest running) order of that method. Thus it is seen that the past performance of the different methods and orders influences the choice of which are allowed to compete, such that the more successful have a higher probability of being selected.

In using the time as the sole estimate of performance efficiency, it is assumed that all orders and methods have satisfactorily met the accuracy requirements. The accuracy requirements of each method are met by controlling step size and making error estimates at each step. The method of error estimate is different for the different methods. In the Runge-Kutta-Shanks single step method, the error is estimated by taking two half steps and then a whole step. In the Adams and Butcher methods the difference between predictor and corrector is used. In the Cowell method a mid-range formula is used. (Only in the Adams and the Runge-Kutta-Shanks cases is there good theoretical justification for using these methods to calculate the actual error -- the error estimates in the Butcher and Cowell methods are essentially empirical.)

### C. Organization of the History File

The history of the effectiveness of each method is recorded in a file called "A831HST" and organized in the following manner.

Associated with each order of each method are two numbers. The first (a positive number) records the time associated with trials in which this order was the winner. The second (a negative number) records the time associated with trails in which it was the loser. The sum of these two numbers is taken as the "score" or performance number and will be greater if the order of this method has been a consistent winner and will be less (more negative) if it has been a consistent loser.

Associated with each method then is a method score analogous to the order scores just described. That is, each method has one positive and one negative number recording the time spent winning and losing respectively. In addition to this, a history is also kept of which methods the wins and losses were against, but this part of the history is not used in selecting competitors.

The history file is printed in an output file called "HISTORY." In describing this, use will be made of an abbreviated notation. A stands for Adams method, B for Butcher, C for Cowell, and S for Shanks formulas. A number given following the letter designates the order of that method where 1 stands for the lowest order available, 2 for the next lowest, etc. Thus A3 stands for the second highest order Adams method. A sign following the letter or number designates winning time or losing time for this method-order. For example, B2 designates winning time for Butcher's method, second lowest order; C designates losing time for Cowell's method; etc. Finally, if a letter follows the sign in parenthesis, this designates which method the win or loss was against; thus B (A) designates winning time by Butcher against Adams. With this notation the organization of the history file is as follows:

The first three items (printed on the first line of the output of the history file) are not times but other bookkeeping items. The first number gives the date (in the form year, day) that this particular history file was initialized, that is the date the tape was first created. The second number gives the total number of times the procedure has been called (using this particular history file). The third number gives the present value of the random number used in generating the random number sequence.

Following these three numbers come the cumulative times the various methods spent winning and losing. These are organized in a 9 row - 8 column matrix. The first 4 rows give wins and losses of the various orders within each method, that is the results of the competitive trials over the 1/8 sections of the range of integration. Table I gives this organization in terms of the notation described above.

Following this is a row giving cumulative winning and losing times by methods; that is, the results of the trials over the 1/4 sections of the range of integration. This row is organized:

$$A^+$$
  $A^ B^+$   $B^ C^+$   $C^ S^+$   $S^-$ 

The last four rows give a more detailed breakdown of the line above, giving the method against which the winning and losing times were made. It is organized as in Table II. It is noted here that entries of the form  $A^{+}(A)$ ,  $B^{-}(B)$ ,  $C^{+}C$ , etc. will all be zero, since methods do not compete against themselves.

TABLE I

ORGANIZATION OF CUMULATIVE WINNING
AND LOSING TIMES BY METHOD AND ORDER

 Al <sup>+</sup>	Al	A2+	A2	A3 <sup>+</sup>	A3 -	A4+	A4-
Bl <sup>+</sup>	Bl -	в2 <sup>+</sup>	B2 -	в3 <sup>+</sup>	B3 -	B4+	B4-
Cl <sup>+</sup>	Cl	C2 <sup>+</sup>	c2 -	c3 <sup>+</sup>	c3 <sup>-</sup>	C/++	C4-
sı <sup>+</sup>	sı-	s2 <sup>†</sup>	s2 -	\$3 <sup>+</sup>	s3 ¯	54+	s4-

Notation here: A = Adams, B = Butcher, C = Cowell, S = Shanks;

1 = lowest order, 2 = second lowest order, etc;

+ stands for win, - stands for loss.

TABLE II

ORGANIZATION OF CUMULATIVE WINNING
AND LOSING TIMES BY METHOD VS. METHOD

A <sup>+</sup> (B)	A <sup>-</sup> (B) A <sup>-</sup> (C)	B <sup>+</sup> (A) B <sup>+</sup> (B) B <sup>+</sup> (C) B <sup>+</sup> (S)	B (B)	$C^{+}(C)$	C (B)	s <sup>+</sup> (c)	s (B) s (C)	
A <sup>+</sup> (S)	A (S)	B <sup>+</sup> (S)	B <sup>-</sup> (S)	C <sup>T</sup> (S)	c_(s)	s (s)	S (S)	

Notation here: A = Adams, B = Butcher, C = Cowell, S = Shanks; + stands for win, - stands for loss.  $A^+(S) \text{ stands for Adams win against Shanks,}$ 

 $C^{-}(B)$  stands for Cowell loss against Butcher, etc.

Entries of the form  $A^+(A)$ , or  $C^-(C)$  etc., should all be zero since a method does not compete against itself.

#### D. Inputs to the Executive Procedure

A call in the executive procedure would look like the following:

DIFEQINT (N, XI, XF, Y, F, P, EA, ER, DX)

Here the identifiers in parenthesis are the inputs to the procedure and represent the following information:

N is the number of equations in the system to be integrated,
XI is the initial value of the independent variable,
XF is the final value of the independent variable.

Y is the initial values of the dependent variables. Y is a vector (one dimensional array). At the conclusion of the procedure Y is set to the final values of the dependent variable; that is, Y is also the output variable.

F is the procedure for calculating dy/dx as a function of x and y. This procedure must be written by the user and describes the system of differential equations being integrated. It must be written so as to have four parameters:

- (a) N, the number of equations,
- (b) X, the independent variable,
- (c) Y, the dependent variable (vector),
- (d) FV, the vector values of dy/dx at the point x, y. The first three parameters are input and FV is the output.

P is the error accumulation parameter. This parameter expresses the user's opinion as to how the errors are going to accumulate over the range of integration. For example, if it is expected that the errors will be  $\underline{\text{random}}$  then P would be set to 0.5. If it is expected that the errors will  $\underline{\text{accumulate}}$   $\underline{\text{linearly}}$  then set P = 1. These are the two most usual cases but other situations can occur.

EA is the absolute error vector. This vector gives the acceptable absolute errors in the value of Y final.

ER is the relative error vector. This vector gives the acceptable relative error in the value of Y final. It is the <u>weaker</u> of the two conditions EA and ER that is met for each component of the vector Y.

DX is the estimated value of the initial step size. This estimate need not be especially accurate since the individual methods will adjust the step size to the appropriate value.

# E. Updating of the History File and Forgetting

The times recorded in the history file are cumulative. That is, after a competition is held, the times taken by the competing methods and orders are added to (for a win) or subtracted from (for a loss) the appropriate positions in the history file. Thus, the entries in the history tables represent an index expressing the cumulative past performance.

Decisions as to which method or order within a method is considered to have the best performance history are made on the basis of the sum of the win and loss entries for that method or order. The method or order having the maximum value for this sum is considered to have best history (remembering that the loss entries are negative). One notes that not all the history file is used in the decision making process; in particular, those entries in Table II are not used in decision making but are recorded only to give the user a more detailed account of the competitions.

One further feature is introduced into the learning process and this is the gradual "forgetting" of events in the more distant past. This is accomplished by multiplying those history scores used in the decision making by a factor less than one, just before the most recent histories are added.

This causes the events in the distant past to have less influence than those more recent in determining the performance figure of an order and method. The factor used is 0.98 but it is not known what would be the optimum factor. Note that the entries in the history file described in Table II do not involve forgetting. Since these entries are not used in any decision making process but only tabulated for the user's interest, forgetting would serve no practical purpose here. The entries in Table II represent then a total or unattenuated history of the competition between the various methods.

## F. Reading of Coefficients and History Files

Also needed as input to the executive routine are the tables of coefficients associated with the various methods and the past performance history file. These are read in to the procedure the first time the procedure is called and a flag set (in an element of an array declared OWN) to indicate that these have been read in once. This information is stored in an array declared OWN and need not be read in again during the operation of the program.

The coefficients are stored on a tape file called "TAPE831." It contains the following coefficients:

Adams'method, orders 4 through 10,
Butcher's formulas, orders 3, 5, 7, 9, 11,
Cowell's method, orders 7, 9, 11, 13,
Shanks formulas, orders 4, 5, 6, 7, 7, 8, 8.

Only four orders of each method are actually used.

The history is stored in a tape file called "A831HST." This tape must be mounted with a write ring and is updated every time the procedure is called.

## G. Outputs of the Executive Procedure

The executive procedure returns the final value of the independent variable as its principal output. This is returned through the same variable, Y (a vector), described in Inputs to the Procedure, paragraph D of this Chapter.

There are several other types of output that are printed. First, when the procedure is called for the first time and reads in the past performance history file, it prints out this history in a print file called "HISTORY".

Also printed out in this file is a pair of numbers giving the method and order that is about to be used and the times for each order and method after the comparisons have been made. This information is printed in a two digit code, the first digit representing the method and the second (if present) indicating the order. The method code is:

- O represents Adams,
- 1 represents Butcher,
- 2 represents Cowell,
- 3 represents Shanks.

The order code is such that 0 represents the lowest order, 1 represents the next lowest order, etc.

Also printed in the file "HISTORY" are the results of comparison runs in which the results (values of the dependent variable) of the two competing method orders differ by more than twice the allowed errors. Also printed are the initial and final values of the independent variable, the two differing values of the dependent variables and an integer telling which component of the dependent variable appears to be in error.

Other messages associated with anomolous conditions are also printed in this file. In particular an integer overflow condition occurs if the step size collapses. Recovery from step size collapse can usually be effected

but the message "INTEGER OVERFLOW" will be printed in file "HISTORY" whenever it occurs.

Finally, the procedure outputs the updated performance history by writing it back into the "A831HST" tape file.

## H. Flow Diagram and Program Listing

Figure 6 is the flow diagram for the executive procedure. The program listing for the executive procedure follows at the end of this section. Since the individual methods and restart programs are also listed elsewhere in this report, their listing here is given in "squeezed" form.

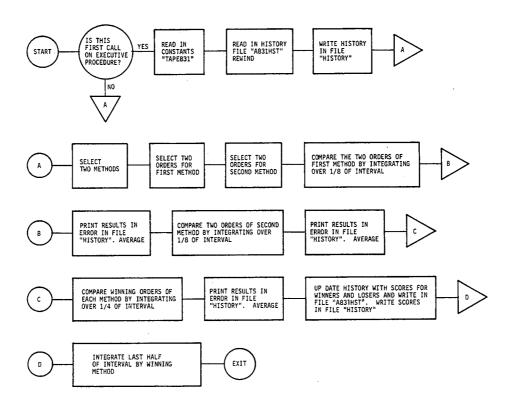


Figure 6. Flow Diagram for the Executive Procedure.

PUN PUNC DURE	00002000
NøXFøXIøDXøP ER Nø	000500
XI, XF DURE	000700
Y YAEAA I #XF T	006000
	001100
K PROCEDURE START(NoxIoxFocisEAsERsfomoxxyivyyHoffsyffocyiocymop Alorksconsiolvaluf noxioxfociomocyiocymopa, poeneval innicorpor	A , 0000
CYMPPAPENEVAL BREAL XIDXFDXPP BREAL ARRAY EADERDYIVDYFVDRKSCONST	000001
*IO * 01 PROCEDURE F \$ BEGIN INTEGER IS JAKALACOEFFONTA FINDX * INDX * NI * DETA * INTEGER * OF * O	ND0000
**************************************	/20000 L60000
EDURE RUNKUTON, XAFNMAXACOEFFATIVATEVAFVAFAGJIVALUE NAXAFNMAX IIN	TE0000 1
'NMAX FREAL X FREAL ARKAY COEFFFYIVFYFVFFV(0)FG(0)OJFPROCEDURE F Integer ijjjkjcont freal temp ftemp (=coefficent (=0))for t (=co	\$0000 1 ST0000 1
NIIL FNMAX DO BEGIN FOR J := 1 STEP 1 UNTIL N DO YFV[J]:=FV[J]XTE	MP0000 1
JIFTOR K ##O STEP 1 UNTIL I #1 DO BEGIN TEMP ##COEFFICONT ##CCNT J ##1 STEP 4 INTIL N OD VEVELIJ##OFK. IJKTEMD LVEVELJEND #FAN. V	+0000
AT #=CCNT +11, YFV, GLIS*1) FTEMP #=COEFFICCNT #=CCNT +11END FFOR J	1 0000:
1 UNTIL N DO YFV[J]:=FV[J]XTEMP +YIV[J]FDR K :=0 STEP 1 UNTIL	F0000 1
JOSEGIN LEMP EMCUEFFICONI EMCONI HIJFFUR JOSHE STEP I UNTIL N DO #G[K>J]xTemp +YFV[J]END FEND /BOOLEAN PROCEDURE COMP(N.FAV.FRV.V	Y0000 1
N FINTEGER N FREAL ARRAY EAV, ERV, Y, ZEOJFBEGIN INTEGER J FREAL	T10000 2
. LI JFOR J ##1 STEP 1 UNTIL N DO IF (T1 ##ABS(YLJ]=ZLJ])>EAVLJ	1T0000 2
4P #BTRUE JELIEND BONTR ##1 PIF M #O THEN BEGIN COFFECNT ##10000	E0000 2
FNEVAL) /2) # FNMAX :=FNEVAL -2 fINT :=XF -XI FTWOH :=(INT +INT	7/0000
FILM /CI FEOR I SEO STEP 1 UNTIL COEFFCNT DO BEGIN HCFIJSECTI S [[1]]XH \$TWOHCFIJSET4 XTWOD END \$TNDX SECX4 NOD 624 \$44.54.64.64	=R0000 2
J ##1 STEP 1 UNTIL N DO BEGIN EAVEJ1#EAEJ1/T1 #ERVEJ1/T	1 0000
PA =2 THEN BEGIN NINDX +=(INDX +1)MOD CYM +K +=0 +GO TO L3 END	30000 2
LI THEN C. SHEMDIV ON SKONNOTONOKAFNMAKATMOHONYIVATIAFHLINDKARJAFA L4 Jelsemoh shembonta shonta shonta soli sholi teli shi shini vot sh	2 00000 S
STEP 1 UNTIL COEFFCNT DO BEGIN TWOHCEIl: #HCEIli#RKSCONSTE	1 10000 3
DX #=CYI MDD CYM #T1 #=(C1 /2)*P #IF PA =2 THEN BEGIN K #=0	\$ N0000 3
• FLINDX • LIMUD CIM JEUR J • HI SIEP I UNIIL N DU BEGIN EAVEJIHEAE	10000

9 64 65 99 29 9 6 0 0 **~** 2 50 90 10 4[J]END ELSE GO TO L1 END END 7X :=M XH +X END 3START :=CNTR 3END 3PROCE0000 DURE ADAMS(N»XI»XF»Y»F»P»Q»DX»EA»ER»ADAMSCOEFF»RKSFNS»RKSORDER»RKSCOEFF»0000 RE F.SHANKSIINTEGER PROCEDURE STARTIBEGIN DEFINE YI#Y#, YB#Y#, YF#Y#, POINTOOOO DIALLI CELI+YPELI+YBELIIIBGOOD+TRUEIEND#SCALLOB#BEGIN SHANKSCNSXXXFSYBSFSOOO RKSFNS, RKSORDER, RKSCOEFF, PLEA, ER, XF "X); END #, ALLMU=FOR MU+OSTEP 1UNTIL OMOOOO INDX +13MOD CYM 3FCN»K XH +X,YHLINDX,\*1,FHLINDX,\*1)3L31RUNKUTCN,K XH +X,0000 FNMAX, TWOHC, YHLINDX, \* 1, Y1, FHLINDX, \* 1, F, G); GU TO L2 END ; IF K #M THEN BEGOOOD IN INDX : #NINDX FF(N\*K XH +X\*YHLINDX\*\*)\*FHLINDX\*\*1)END END ELSE GO TO L10000 END ELSE BEGIN FOR J 1=1 STEP 1 UNTIL N DO BEGIN EAVEJ]: = EALJJ71 JERVEDDO JI: #EREJJ/TI 3Y1EJJ: #Y2EJJEND 3L4: RUNKUT(N» X»FNMAX»HC»YIV»Y2»FHEINDX»\*1,0000 Fog) INDX 1 = (INDX +1) MOD CYM FF(N, X +H, Y2, FH[INDX, \*1) FRUNKUT(N, X +H, FNMA0000 XAHCAY2AY4AFHLINDXA\*1AFAGAK 1=2 FIF PA =0 THEN BEGIN LSTIF COMP(NAEAVAE0000 RV, Y1, Y4) THEN BEGIN IF K <M THEN BEGIN INDX \$=(INDX +1)MOD CYM 3F(N, K XHOOOO +X»Y4»FH[INDX»\*])\$RUNKUT(N»K ×H +X»FNMAX»TWOHC»Y4»Y1»FH[INDX»\*]»F»G)\$RU0000 NKUTCN.K XH +X.FNMAX.HC.V44.Y3.FHLINDX.\*1.F.G.).K :=K +1 JINDX :=(INDX +1)0000 MOD CYM JF(NoK XH +XoY3oFH[INDXo\*1)JRUNKUT(NoK XH +XoFNMAXoHCoY3oY4oFH[I0000 OD CYM JF(N.K XH +X,Y4,FH[INDX,\*]);FOR J :=1 STEP 1 UNTIL N DO YFV[J];=Y0000 4[J]END ELSE FOR J 1=1 STEP 1 UNTIL N DO YFV[J]1=Y3[J]END ELSE GO TO L1 0000 END ELSE BEGIN L6:1F COMP(N,EAV,FRV,Y1,Y4)THEN BEGIN INOX :#(INDX +1)MOD0000 CYM JECNOK XH +XoY40FHCINDXo+1)JIF K. <M THEN BEGIN IF K =L THEN FOR J 10000 #1 STEP 1 UNTIL N DO YFV[J]: #Y4[J];RUNKUT(N,K XH +X,FNMAX,TWOHC,Y4,Y1,FH0000 IINDX\*\*1,F&G);RUNKUT(N\*K XH +X&FNMAX&HC&Y4&Y3&FHLINDX\*\*1,F&G);K %=K +1 30000 INDX :=(INDX +1)MOD CYM SF(N»K xH +X»Y3»FH[INDX»+]) IF K =L THEN FOR J :0000 #1 STEP 1 UNTIL N DO YFV[J]1#Y3[J]1RUNKUT(N.K XH +X.FNMAX.HC.Y3.Y4.FH[IN0000 DX\*\*1\*F\*G) #K +1 #GO TO L6 END #FOR J :=1 STEP 1 UNTIL N DO YIVEJI:=Y0000 START » SHANKS ) I VALUE N » XI » XF » P » Q » D X » RKSFNS » RKSORDER I REAL XI » XF » P » D X I INTEGOOOO ER N.O.RKSFNS, RKSORDERIREAL ARRAY Y, EA, ER, ADAMSCOEFF, RKSCOEFF (01) PROCEDUODOO ART(NoxIoxFoctoEAsERofoRnusiox, yrofhofhoyrojoatemiopoporksfnsorkscoeffoodo INUSI DO# ALLI=FOR I + 1STEP 1UNTIL N DO# » RESET=BEGIN DC+0 PC + Q 1 CU + (C1 + ( + P0000 ))×GRJH+INTERVAL/C1JALLMU BEGIN HB[MU]+B[MU]×HJHBS[MU]+BS[MU]×HJENDJHBSQOOOQ Z+BSQZ×HJALLI BEGIN EAL[1]+(EAU[1]+EA[1]xcU)xC2MQP5JERL[1]+(ERU[1]+ER[1]0000 xCU)xC2MQP5;HAL[I]+ABS(EAL[I]/HBSQZ);HRL[I]+ABS(ERL[I]/HBSQZ);END;END#;L0000 ABEL RESTART, NEXTSTEP, FLIP, FLOP, TEST, DUBBLE, HALF, FINISH, FREAL ARRAY FHLO:0000 /TI JERVIJI:=ERIJJ/TI JY1[J]:=YHININDX;JERU JLZ:RUNKUTIN,K xH +X,FNMAX,0000 I=(INDX +1)MGD CYM JF(NJK XH +XJYHLINDXJ\*IJFHLINDXJ+1)JRUNKUT(NJK XH +XJ0000 FNMAX&HC&YHLINDX&\*1,YH[NINDX&\*1,FH[INDX\*\*1,F&G)}IF COMP(N&EAV&ERV&Y1,PYH10000 VINDX\*\*1)THEN BEGIN K :=K +1 !IF K <M THEN BEGIN INDX :=NINDX ; INDX HCAYHLINDXA\*JAYHENINDXA#JAFHLINDXA\*JAFAGAAA 8#K +1 JINDX 8#NINDX BNINDX

(2×Q=2),01N],B,BS,HB,HBS[0:Q=1],C,YP,YC,YD,FP,FC,EAU,EAL,ERU,ERL,HAL,HRL0000 74 [O:N]; REAL HoxoCU, C20 GRoYCIOBSQZoFHJIOFMUIOHBMUOM1DPOHBSMUOHBSQZOERROR, COOOO 75 HANGE, C2MQP5, INTERVAL; INTEGER I, J, K, C1, DC, PC, MU, MULT, JZERO, QT2M1, QMINUS10000 76 QTIMES23BOOLEAN BGOOD, FLIPPED, TOOSMALL3C2MQP5+1/2\*(Q+5)3QMINUS1+Q-13QTIOOOO 77 MES2+Q+Q;QT2M1+QTIMES2-1;ALLMU BEGIN BEMUJ+ADAMSCOEFFEMUJ;BSEMUJ+ADAMSCOOOO 78 EFF[MU+Q]; END; BSQZ+ADAMSCOEFF[QTIMES2]; GR+ADAMSCOEFF[QTIMES2+1]; C1+1; H+TOOOO 79 NTERVAL+XF\*XI3DX+ABS(DX)3WHILE ABS(H)>DX OR C1<Q DO BEGIN C1+C13H+INTOOOO 80 ERVAL/C1; END; C2+C1; JZERO+J+O; F(N, XI, YI, FH(O, +)); X+XI; ALLI YB[I]+YI[I]; BGOOOO 81 OOD+TRUE; RESTART: POINTS; C1+C1×MULT; C2+C2×MULT=Q; IF(J+JZERO=1)<OTHEN J+J+0000 82 QT2M1;RESET;NEXTSTEP:X+XF=C2×H;ALLMU BEGIN IF(J+J+1)=QT2M1 THEN J+0;HBMU0000 83 +HB[MU];HBSMU+HBS[MU];ALLI BEGIN YP[I]+(FMUI+FH[J,[])×HBMU+YP[I];C[I]+HB0000 84 SMU×FMUI+C[]];END;END;F(N,X,YP,FP);FLIP;ALLI YC[]]+FP[]]×HBSQZ+C[]];F(N,0000 85 X,YC,FC);ALLI IF(CHANGE+ABS(FC[I]=FP[I]))>HAL[I]THEN IF CHANGE>ABS(HRL[I0000 86 JXFC[I]) THEN GO TO FLOP; FLIPPED+TRUE; GO TO TEST; FLOP; ALLI YC[I]+FC[I]XHBOOOO 87 SQZ+C[I];F(N,X,YC,FP);ALLI IF(CHANGE+ABS(FP[I]=FC[I]))>HAL[I]THEN IF CHADOOD 88 NGE>ABS(HRL[I]×FP[I])THEN GO TO FLIP;FLIPPED+FALSE;TEST:IF(J+J+1)=QT2M1 0000 89 THEN J+01T00SMALL+TRUE1ALLI BEGIN FHJI+FH[J,I]+IF FLIPPED THEN FC[I]ELSF0000 90 FP[I]JERROR+ABS(YP[I]=(YCI+C[I]+YP[I]+(FHJI×HBSQZ+C[I])))JTF BGOOD THENOOOO 91 YD[I]+YCI ELSE YB[I]+YCI;YCI+ABS(YCI); F ERROR>EAU[I]THEN IF ERROR>ERU[0000 92 I] × YCI THEN GO TO HALF; IF ERROR > EAL[I] THEN IF ERROR > ERL[I] × YCI THEN TOOSOOO 93 MALL+FALSEJENDJPC+PC+1JIF BGOOD THEN BGOOD+FALSE ELSE BGOOD+TRUE; IF C2≥10000 94 .OTHEN C2+C2-1.OELSE GO TO FINISH; IF TOOSMALL THEN BEGIN DC+DC+1; IF DC>30000 95 THEN IF PC≥QT2M1 THEN IF C2≥1THEN GO TO DUBBLEJIF(JZERO+(J+JZERO)+1)=QT20000 96 M1 THEN JZERO+OJGO TO NEXTSTEPJENDJDC+OJIF(JZERO+(J+JZERO)+1)=QT2M1 THENOGOO 97 JZERO+OJGO TO NEXTSTEPJDUBBLE:C1+C1 DIV 2JC2+(C2-1.0)/2.0JRESETJK+JJFOROOOO 98 MU+1STEP 1UNTIL QMINUS1 DO BEGIN IF(J+J=1)<0THEN J+J+QT2M1; IF(K+K=2)<0T0000 99 HEN K+K+QT2M13ALLI FH[J,I]+FH[K,I];END;IF(J+(JZERO+J)=1)<OTHEN J+J+QT2M10000 100 JGO TO NEXTSTEP; HALF : IF (J+J=1) < OTHEN J+J+QT2M1; JZERO+J; C1+C1; IF (C2+C20000 101 +C2+2.0)<Q THEN GO TO FINISH; GO TO RESTART; FINISH; IF NOT FLIPPED THEN ALOGOD 102 LI FC[I]+FP[I]; IF NOT BGOOD THEN ALLI YB[I]+YD[I]; X+XF-INTERVAL×(C2/C1);0000 103 IF C2 # OTHEN CALLOBJALLI YF[I] + YB[I] JENDJPROCEDURE BUTCHER(N, XI, XF, K, EA, E0000 104 R, DX, CON, FUNCTION, EX, RKC, START, SHANKS, YIV, RKSNF, RKSODR); VALUE N, XI, XF, K, 0000 105 DX, CON, EX, RKSNF, RKSODR, REAL ARRAY YIV[0], INTEGER RKSNF, RKSODR, INTEGER N, 0000 106 KIPROCEDURE FUNCTION, SHANKS INTEGER PROCEDURE STARTIREAL XI, XF, DX, EXIREA0000 107 L ARRAY RKC[0]; REAL ARRAY CON, EA, ER[0]; BEGIN REAL ARRAY Y, F[0:16,0:N]; RE0000 108 AL SC1, X; REAL DX2; REAL DX1, COA, COB, COLA, COLB, COGA, COGB, TEST, TEMPY, TEMPF, 0000 109 A1, A2, A3, C2, INTEGER I, J, CYL, INDEX, C1, M, INTEGER CYL3, REAL ARRAY SUMYIP, SU0000 110 MYP, SUMYC, FV1[0:N]; LABEL STRRT, RESTART, FINISH; REAL P2, T1, T2; INTEGER COUNOOOO 111 EGER COUNTER; INTEGER KM1; REAL OMT, K6, K61, K62; REAL INTV; INTEGER KM3, J2, J30000 113

JOJREAL XDXT, XDXJREAL ARRAY RE, AE(O:N]JFOR I+1STEP 1UNTIL N DO Y[O, 11+Y0000 114 IV[I]] IF K=10R K=20R K=3THEN OMT+0.5ELSE OMT+2/38K6+6×KJK61+(6×K)+1JK62+0000 115 (6×K)+2JKM1+K=1JINTV+XF=XTJX+XTJC1+1JWHILE(C1<K+1)OR(CABS(INTV)/C1)>ABS(OOOO 116 DX))DB C1+C1+C1+C2+C1+P2+1/(2\*((2\*K)+4))+CYL+O+CYL+O+TOTCNT+O+FUNCTION(NOOOO 117)aXIaYfOa\*laFfOa\*ll}RESTART&COUNTER&KM1;C1&C1XCI&START(NaXIaXFaC1aEAaERaFOOOO 118 UNCTION, KM1, X, YIV, Y, F, YIV, CYO, 16, 2, EX, RKSNF, RKC)); C2+C2×I+KM1; CYL+CYO; DUOOOO 119 BSRT:DX+INTV/C1;KM3+3×KM1;FOR J+OSTEP 3UNTIL KM3 DO BEGIN J2+2×J;COO[J]+0000 120 CON[J2+1]\*DXJCOO[J+1]+CON[J2+3]\*DXJCOO[J+2]+CON[J2+5]\*DXJENDJSC1+C1\*EXJF0000 121 OR I+1STEP 1UNTIL N DO BEGIN AELT1+EACIJ/SC13RECIJ+ERCIJ/SC13END3A1+CONCOOO 122 K6]×DXJA2+CON[K61]×DXJA3+CON[K62]×DXJSTRRT:XDXT+X+(DX×OMT)JXDX+X+DXJFOR 0000 123 I+1STEP 1UNTIL N DO SUMYTP[I]+SUMYP[I]+SUMYC[I]+O;FOR J+OSTEP 1UNTIL KM10000 124 DO BEGIN CYL3+(KM1=J+CYL)MOD 161J3+3×J1J6+6×J1COA+CON[J6]1COB+COO[J3]1COOO0 125 OLA+CON[J6+2];COLB+COO[J3+1];COGA+CON[J6+4];COGB+COO[J3+2];FOR [+1STEP 10000 126 AXTEMPY)+(COBXTEMPF);SUMYP[T]+SUMYP[]]+(COLAXTEMPY)+(COLBXTEMPF);SUMYC[]OOOO 128 ] + SUMYC[I] + (COGA×TEMPY) + (COGB×TEMPF) JENDJENDJFUNCTION(N, XDXT, SUMYIP, FV1)0000 129 FOR I+1STEP 1UNTIL N DD BEGIN TFMPF+FV1[I]/SUMYP[I]+SUMYP[I]+(A1×TEMPF)0000 130 JSUMYC[I]+SUMYC[I]+(A2×TEMPF)JENDJFUNCTION(NDXDXDSUMYPDFV1)JCYL+(CYL+1)M0000 131 OD 16JCYO+(CYL+KM1)MOD 16JCOUNT+OJFOR I+1STEP 1UNTIL N DO BEGIN TEMPY+SU0000 132 MYC[T]+(A3×FV1[I]);T1+AE[T];T2+ABS(RE[I]\*TEMPY);TEST+ABS(TEMPY=SUMYP[I])0000 133 JIF TEST>T1 AND TEST>T2 THEN BEGIN C2+C2+C2JCYL+(CYL+15)MOD 16JCYO+(CYL+0000 134 KM1)MOD 1611F C2<KM1 THEN BEGIN SHANKS(NoXoXFoY[CYOo\*]oFUNCTIONORKSNFORKOOOO 135 SODR, RKC, EX, EA, ER, DX), JGD TO FINISH, END, C1+C1+C1, JGD TO RESTART, END, YCCYO, OOOO 136 I]+TEMPYJIF TEST<P2×T1 OR TEST<P2×T2 THEN COUNT+COUNT+1JENDJC2+C2=1JX+XF0000 137 -(DX×C2); IF C2=OTHEN GO TO FINISH; IF C2<1THEN BEGIN SHANKS(NoxoXFoYECYO,0000 138 \*],FUNCTION, RKSNF, RKSODR, RKC, EX, EA, ER, DX) JGO TO FINISH JEND JFUNCTION (N, X, 0000 139 YECYO≠\*J≠FCCYO≠\*J)≯IF COUNT=N THEN BEGIN TOTCNT+TOTCNT+1≯IF TOTCNT≥3THENOOOO 140 BEGIN IF COUNTER≥2×K THEN BEGIN COUNTER+0JC2+C2/2JC1+C1/2JIF C2<1THEN B0000 141 EGIN SHANKS(NaXaXFaY[CYOa+]aFUNCTIONaRKSNFaRKSODRaRKCaEXaEAaERaDX)3GO TOOOOO 142 FINISHJENDJTOTCNT+03FOR 1+1STEP 1UNTIL N DO FOR J+1STEP 1UNTIL KM1 DO BOOOD 143 EGIN CYL1+(CYO+16-J)MOD 161CYL2+(CYO+16-(2×J))MOD 161YICYL1,I1+YICYL2,I10000 144 3F[CYL1¤I]+F[CYL2¤I];END\$GO TO DURSRT;END;END;END;COUNTER+COUNTER+1;GO TOOOO 145 O STRRTJFINISH:FOR I+1STEP 1 UNTIL N DO YIV[I]+Y[CYO,I]JEND BUTCHER;PROCOOO0 146 EDURE COWELL(N, XI, XF, Y, F, EA, ER, P, DX, RKSFN, RKSORDER, RKSCOEFF, Q, COWELL COEFOOOD 147 FOSTARTOSHANKS) JVALUE NOXIOXFOPODXORKSFNORKSORDEROQ JINTEGER NORKSFNORKSOOOO 148 ORDERAQ FREAL XIAXFAPADX FREAL ARRAY YAEAAERARKSCOEFFACOWELLCOEFFCOJFROOOOO 149 CEDURE FOSHANKS SINTEGER PROCEDURE START SBEGIN INTEGER C1. M. MM1. QP1. TQP0000 150 1. INDX, II. IZ. I3, I. J. K. CYT JINTEGER CORRECTONT JREAL INT. C2. DFACTOR, X. H. TOOOO 151 10T20T30T40T50T6 3BOOLEAN DFLAGOPFLAG JREAL ARRAY FHEORQ +QOORNJOYMID10Y0000 152 PayCayMacsaffaHDM1faHDM1fmIDaEAVaERVDeRVDeRVD[0:N]aPCDEFfaCCDEFfaMCDEFF0000 153

9 8 63 9 UNTIL N DO BEGIN EAVD[J]:=(EAV[J]:=EA[J]/T1]/DFACTOR ;ERVD[J]:=(ERV[J]:0000 =ER[J]/T1)/DFACTOR END ;T1 :=MCDEFF[0];FOR J :=1 STEP 1 UNTIL N DO HDM1F0000 N CYI :=(INDX :=(INDX +1)MDD TQP1)+TQP1 8X :=XF -(C2 -I)xH 311 :=(CYI -10000 T4 +T2 ×T3 END \$I3 :=CYI =QP1 \$FOR K :=2 STEP 1 UNTIL M DO BEGIN I1 :=(C0000 YI -K)MOD TQP1 \$I2 :=(I3 +K)MOD TQP1 \$T1 :=PCOEFFIK =11\$T2 :=CCOEFFIK]\$T0000 3 :=PCOEFFIQ =K]\$T4 :=CCOEFFIQP1 =K]\$FOR J :=1 STEP 1 UNTIL N DO BEGIN Y0000 LAG :=TRUE ; CORRECTCNT :=CORRECTCNT +1 ; GO TO L2 END END ; F(N,X,YC,FH[IN0000 DX,\*]); PFLAG :=FALSE ; L2:END ; I1 :=(CYI =M)MOD TQP1 ; T1 :=MCOEFF[M]; FOR 0000 SEXF =XI &C1 S=1 }LOSC1 S=C1 +C1 FIF C1 <0 THEN GO TO LO FIF DX <0 THEN 0000 DX S==DX FIF DX ≠0 THEN BEGIN LISIF ABS(INT)/C1 >DX THEN BEGIN C1 S=C1 +0000 C1 3GD TO L1 END END 3C2 1 = C1 3M 1 = Q DIV 2 3MM1 8 = M - 1 3QP1 8 = Q +1 3TQP10000 +0 JDFACTOR 1=2.0 +(0 +3); INDX 1=0 3X 8=XI JF(N»X»Y»FH[O»+1); STAR0000 JI: #YMID1[J] #FH[INDX > J] X 1 3 CYI SEINDX + TOP1 3 I3 SECYI # OP1 3 FOR K SE1 0000 \*#MCDEFF[K]-H 3T2 \*#MCDEFF[QP1 "K]\$FOR J \*#1 STEP 1 UNTIL N DO HDM1F[J]10000 M DO BEG10000 )MOD TOP! FIL : #PCOEFF[0]; T2 : #CCOEFF[1]; FOR J : #1 STEP 1 UNTIL N DD BEGOOOD IN YP[J]:=(T4 :=(HDM1F[J]:=HDM1F[J]+H x(T3 :=FH[I]+J])))+T1 xT3 ;CS[J]:=0000 N BEGIN IF T1 >ERV[J]xABS(T3)THEN BEGIN FOR J :=J +1 STEP 1 UNTIL N DO Y0000 C[J]:=CS[J]+T2 xFP[J]}F(N,x,YC,FP)}FOR J :=1 STEP 1 UNTIL N DO IF (T1 :=0000 JJSCORRECTONT \$=CORRECTONT +2 JIF CORRECTONT >8 THEN BEGIN INDX \$=(CYI -0000 I) MOD TOP! JGD TO LS END JGD TO CORRECT END END JFCN, X, YP, FHIINDX, + 1) JPF0000 J :=1 STEP 1 UNTIL N DO YMEJI:=HDM1FMIDEJI+T1 XFHEI1+JJ113 1=CYI -Q 1FDR0000 DO BEGIN II 1#(CYI #K)MOD TOP1 312 1#(I3 +K)MOD 0000 TERICL :#(II : #START(N) XI » XF » C1 » EA » ER » F » Q » X » Y » F H » F H » Y MID1 » I ND X » TQP1 » 1 » P » 0000 V PCOEFFIK1: #COMELLCOEFFIK1xH \$CCOEFFIK18 #COMELLCOEFFI11 8#K #QP11xH \$MC0000 DEFFINITECOMELLCOEFFILI + OP13xH END \$71 1=(C1 +P)x10,0 FOR J 1=1 STEP 10000 P[J] t = YP[J] + T1 x(T5 t = FH[I1, J]) + T3 x(T6 t = FH[I2, J]) + CS[J] t = CS[J] + T2 x T5 0000 +T4 xT6 END END 311 1=(CYI =Q)MOO TQP1 312 1=(CYI =QP1)MOD TQP1 3T1 1=PC0000 DEFFIG -11172 := CCDEFFEQ1173 := PCDEFFEQ11FOR J := 1 STEP 1 UNTIL N DO BEGOOOD IN YP[J]:#YP[J]+T1 x(T4 :#FH[I],J])+T3 xFH[I2,J];CS[J]:#CS[J]+T2 xT4 END0000 JT2 ##CCDEFF[0]JCDRRECTCNT :=1 JCDRRECT:F(N,X,YP,FP)JFDR J :=1 STEP 1 U0000 NTIL N DO IF (T1 1=ABS((T3 1=(YCLJ)1=CSLJ)+T2 xFPLJ))-YPLJJ)>EAVLJJTHE0000 ABS((T3 im(YP[J]imcS[J]+T2 xFP[J]))"YC[J])>EAV[J]THEN BEGIN IF T1 >ERV[0000 J1xABS(T3)THEN BEGIN FOR J := J +1 STEP 1 UNTIL N DO YP[J]:=CS[J]+T2 xFP[0000 KKSFNøRKSCOEFF))×C1 3C2 3mC2 ×I1 mg 3INDX 3m(INDX +Q)MDD TQP1 3IF C2 <M 0000 HEN GO TO CLOSER FOOUBLER:H 8=INT /C1 FFOR K 1=0 STEP 1 UNTIL Q DO BEGIO000 J ## STEP 1 UNTIL N DO YMEJ10000 STEP 1 UNTIL M DO BEGIN II :=(CYI -K)MOD TOP1 !IZ :=(I3 +K)MOD TOP1 !TI LO>L1>L2>L3>L4>L5>STARTER, DOUBLER, ACCEPT, CORRECT, CLOSER, INT UNTIL UNTIL tat STEP =HDM1F[J]=FH[I1.J]×I1 =FH[I2.J]×T2 END FFOR J :=1 FMIDEJ1:#HDM1FEJ3DFLAG :#FALSE ;ACCEPT:FOR I SHMCDEFFEG -KJJFOR OP1 JT1 8=MCDEFF[K]JT2 K := 0 STEP 1 UNTIL MM1 8 # Q P 1

\$=YM[J]+T1 ×FH[I1₀J]+T2 ×FH[I2₀J]END \$IF DFLAG THEN BEGIN FOR J :=1 STEP0000 194 1 UNTIL N DO IF (T2 %=ABS((T3 %=Y[J])-YM(J]))>FAVD(J]THFN BFGIN IF T2 >0000 195 ERVD[J]×ABS(T3)THEN BEGIN IF T2 >EAV[J]THEN BEGIN IF T2 >ERV[J]×ABS(T3)T0000 196 HEN GD TO L4 END 3GO TO L3 END END 3C2 1=C2 PM 3C2 1=C2 /2.0 3IF PFLAG TOOOD 197 HEN FOR J :=1 STEP 1 UNTIL N DO YEJ]:=YPEJJELSE FOR J 8=1 STEP 1 UNTIL NOOOD 198 DO Y[J]: #YC[J]; C1 :=C1 DIV 2 ; IF C2 < M THEN GO TO CLOSER ; INDX :=INDX +0000 199 1 FOR K #=1 STEP 1 UNTIL Q DO BEGIN INDX :=(INDX +1)MOD TQP1 FI1 :=(IND0000 200 X +K)MOD TQP1 FOR J == 1 STEP 1 UNTIL N DO FHEINDX,J] = FHEI1,J]END JGD TOOOD 201 O DOUBLER END \$J \$=0 \$L3&FOR J \$=J +1 STEP 1 UNTIL N DO IF (T2 \$=ABS((T30000 202 \*=Y[J]) TYM[J]))>EAV[J]THEN BEGIN IF T2 >ERV[J]×ABS(T3)THEN BEGIN L4\*IND0000 203 STARTER END END ≯C2 :=C2 =M ≯IF C2 ≥M THEN BEGIN IF PFLAG THEN FOR J :=10000 205 STEP 1 UNTIL N DD BEGIN YMID1[J]:=Y[J];Y[J]:=YP[J];HDM1FMID[J]:=HDM1F[J0000 206 JEND ELSE FOR J #=1 STEP 1 UNTIL N DO BEGIN YMID1[J]#=Y[J]#Y[J]#=YC[J]#H0000 207 DMIFMIDEJ] = HDMIFEJJEND & DFLAG = TRUE & GO TO ACCEPT END & IF PFLAG THEN FOOOD 208 OR J :=1 STEP 1 UNTIL N DO Y[J]:=YP[J]ELSE FOR J :=1 STEP 1 UNTIL N DO Y0000 209 [J]:=YC[J];CLOSER: C2 >0 THEN SHANKS(NoXoXFOY)FORKSFNORKSORDERORKSCDEFO000 210 FOPAEADEROABS(INT)/C1)JEND JPROCEDURE SHANKS(NAXIDXFOYVOFOMOORDEROCFOPOE0000 211 A.ER.DX); VALUE N.XI.XF.M.ORDER.P.DX; INTEGER N.M.ORDER; REAL XI.XF.P.DX; RE0000 212 AL ARRAY YV.CF.EA.ER[0];PROCEDURE F;BEGIN INTEGER I.J.K.L.COUNT.COUNT2.10000 213 I, NCF JINTEGER NCF 1 JINTEGER DKTR JREAL EFACT JREAL BETA, DCDUNT, DXD, DXH, DXT, 0000 214 EFACTOR, ERANGE, ES, GAMMA, X, XM, BOOLEAN CFSW, DSW, REAL ARRAY CFDEO: (M+3)×M=20000 215 ], FV[0:M=1,00:N], GVpYCpYMpYP[0:N]; DEFINE CFH=CFD#; LABEL L1, L2, EXIT; INTEGEO000 216 R STEPRISTEPSIM+M=1;STEPS+STEPR+0;DXD+DXT+XF=XI; IF DXT=0THEN GO TO EXIT;0000 217 TF DX=OTHEN DX+DXDJCOUNT+1JWHILE ABS(DX)<ABS(DXD)DO BEGIN COUNT+COUNT+CO0000 218 UNTIDXD+DXT/COUNTIENDICOUNT2+COUNT+COUNTIDXH+DXT/COUNT2IDCOUNT+COUNTIEFA0000 219 CT+13FOR I+1STEP 1UNTIL ORDER DO EFACT+EFACT+EFACTJERANGE+0.125/EFACTJEF0000 220 ACT+4/EFACTJEFACTDR+COUNT\*P×EFACTJDKTR+0JNCF1+(M×M+M)DIV 2+M+MJNCF+NCF1+0000 221 1)CFSW+FALSEJFOR I+OSTEP 1UNTIL NCF1 DO BEGIN CFD[I]+CF[I]\*DXDJCFH[I+NCF0000 222 ]+CF[I]×DXH;END;X+XT;XM+XT+DXH;L1:DSW+TRUE;F(N,X,YV,GV);IF CFSW THEN L+N0000 223 CF1 ELSE L+-13FOR I+1STEP 1UNTIL M DO BEGIN II+I-13L+L+13BETA+CFD[L]3FOR0000 224 K+1STEP 1UNTIL N DO YP[K]+GV[K]×BETA+YV[K])FOR J+1STEP 1UNTIL II DO BEGOOOD 225 IN L+L+13BETA+CFD[L]3FOR K+1STEP 1UNTIL N DO YP[K]+FV[JoK]×BETA+YP[K]3EN0000 226 DJL+L+13F(N,CFD[L]+X,YP,FV[],+])JENDJL+L+13GAMMA+CFD[L]3FOR K+1STEP 1UNT0000 227 IL N DO YP[K]+GV[K]×GAMMA+YV[K];FOR I+1STEP 1UNTIL M DO BEGIN L+L+1;GAMM0000 228 A&CFD[L])FOR K+1STEP 1UNTIL N DO YP[K]&FV[],K]XGAMMA+YP[K])END)L2:IF CFS0000 229 W THEN L+=1;FOR I+1STEP 1UNTIL M DO BEGIN II+I=1;L+L+1;BETA+CFH[L];FOR K0000 230 +1STEP 1UNTIL N DD YM(K]&GV[K]×BFTA+YV[K];FOR J+1STEP 1UNTIL II DD BEGINOOOD 231 L+L+1/BETA+CFH[L]/FOR K+1STEP 1UNTIL N DO YM[K]/FV[J/K]XBETA+YM[K]/END/0000 232 L+L+13F(NoCFH(L)+XoYMoFV(No+1)3END3L+L+13GAMMA+CFH(L)3FOR K+1STEP 1UNTIL0000 233

```
00025000
                                     OMN INTEGER KX, KY, KX33, KX41, KY33, KY41,
00057000
                                                 OWN INTEGER ARRAY Q1-2:7333
00023000
                                               DMN ARRAY CUEF[0:3,0:3,0:39]
00022000
                                                               BEAL A.C.DUXF
00051000
                               ENEMAT FM5110 (4(211,18,X2),2(11,18,X2),110)
00002000
                                                   DEFINE SS =START, SHANKS#3
00061000
                 ×BBS(Y [J]+Y1[J])THEN WRITE(PUN FF4E11AACAY1[J]AY [J]AJ)#}
DEFINE AC =ALLJ IF (TEMP :=ABS(Y [J]=Y1[J])>EA[J]x2 AND TEMP >ER[J]00018000
00011000
                                                                  REAL TEMP3
00091000
                                                    EUKMAT F4E11(4E20,9,19))
00051000
                                                           FURMAT F211(211)}
00011000
                                                                  TVRET: T361
00013000
                                  INTEGER OVERFLOW") !
                                                           FORMAT FMINTOVR("
00015000
                                                             MONITOR INTOVRS
                                               NIIF NCEI DO CED[I+NCE] + CE[I] × DXDICE2M + LKNEIENDIENDIXM + (CONNIS+I=DCONNI=0000 520
INNIIT NCEI DO CEDIII+CELIIXDXDICERM+EVTREIEND ETRE BEGIN EOK I+ORIES INOOOO 521
+DXD}DXD+DX1\COON1}EEVCLOB+COON1+b×EEVCL}IE CE2M THEM BEGIM EOB I+O21Eb 0000 520
HEN BEGIÑ DKIK←DKIK+IlCONNIS+CONNIlCONNI CONNI DIN SIDCONNI←DCONNI\SIDXHOOOO 522
ERIN CED[I]+CE[I]×DXD}CEH[I+NCE]+CE[I]×DXH}END}RO 10 FI}END}END}IE DRM 10000 $2¢
XD←DXI←XE=XI}DXH←DXD\S}XW←XI+DXH}CE2M←EFF2E1EDB I←021Eb 1AAIIF NCE1 DO 80000 S23
IE DCOONI>TIHEN DKIK+DKIK+TYCOONI+DCOONI+TYCOONIS+SYEEVCLOK+EEVCLYXI+XYD0000 525
ONNI<SIHEN BEGIN IL DCONNI≃IIHEN D8M←LVΓSEIIL DCONNI<IOB D2M IHEN BEGIN 0000 521
DO YVIKJ +YCIKJJIF DCOUNT=OTHEN GO TO EXITJX+(COUNT-DCOUNT)×DXO+XIJIF DC0000 250
HEN DOM+FALSEJENDJENDJDCOUNT+DCOUNT=1JSTEPS+STEPS+1JFOR K+1STEP 1UNTIL NOOO0 249
PENDVIE DRW THEM IE ESSER[K]×EKRMGE THEM IF ESSABS(YC[K])×ER[K]×ERMGE T0000 248
NIS+I∞DCONNI=DCONNI)×DXH+XI}ENK K←IZIEL INNIIF N DO AL[K]←AW[K]}€O ±O 「SOOOO S∀L
BECIN LOW I←021EL INNIIT NCLI DO CLH[I]+CL[I]×DXH1CL2M←1BNE1END1XM←(CON0000 5de
EGIN LOB I←OZIEЬ INNIIT NCLI DO CEH[I+NCL]←CE[I]×DXH}CEZM←EBTZE}END ETZEOOOO $∀⊋
CONNI+DCONNI}DXD+DXH}DXH←DXI\CONNIS}EE∀C108←CONNI+b×EE∀C1}IE CE2M IHEN B0000 $dd
N BEGIN D2M←E∀F2E121EbK+21EbK+11CONN1<CONNIS1CONNIS←CONN1+CONN11DCONN1¢D0000 5¢3
[K])×EFACTOR}IF ES≠OTHEN BEGIN IF ES≥EA[K]IHEN IF ES≥ABS(YC[K])×ER[K]THEO000 242
KI+EN[I*K]×GAMMA+YC[K];ENDJFOR K+1STEP 1UNTIL N DO BEGIN ES+ABS(YC[K]-YP0000 241
I+021EP 1UNTIL M DD BEGIN L+L+11GAMMA+CFH(L)1FDR K+15TEP 1UNTIL N DD YC(0000 240
1}E(N>CEH[F]+XW>XC>EN[I>*])}END}EOB K←121Eb 1NNIIF N DO XC[K]+XW[K]}EOB 0000 530
+J}BEIA←CEH[[]}EOK K←JZIEb JONII[ N DO XC[K]←EN[¬ႃK]×BEIA+XC[K]}END}[←[+0000 S38
1}ŁOB K←121EB 1NNIIT N DO XC[K]←XW[K]}ŁOB 7←021EB 1NNIIT II DO BECIN T←Γ0000 531
A[O>*]); IE CESM THEN LETSE LENCELIFOR IFISTEP 1UNTIL M DO BEGIN II+1=0000 236
CEH[୮]}EOB K←12IEb 1NMIIT N DO XW[K]←EN[I³K]×C¤WW∀+XW[K]}END}E(N³XW³XW³E0000 532
N DO XWEKJ+GVEKJ×GAMMA+YVEKJJFOR I+1STEP 1UNTIL M DO BEGIN L+1JGAMMA+0000 234
```

```
DWN INTEGER J.S.K.
                                                                          00026000
DWN INTEGER ARRAY AT BJ[083]
                                                                          00027000
                                                                          00028000
LIST LST(FOR J:==2 STFP 1 UNTIL 72 DO Q[J]);
DEFINE HEREBEFORE =Q[73] ##ALLJ =FOR J == 1 STEP 1 UNTIL N DO ##YOBYY 00029000
=ALLJ YO[J] = Y[J] # SFTY1ANDY = ALLJ
                                                                          00030000
BEGIN
                                                                          00031000
  Y1[J]:=Y[J];
                                                                          00032000
  [L]OY=:[L]Y
                                                                          00033000
END #3
                                                                          00034000
LABEL L290L10L20L30L40L50L60L70M000M010M020M030M100M110M120M130M200 00035000
M21, M22, M23, M30, M31, M32, M33;
                                                                          00036000
SWITCH SW ==M00,M01,M02,M03,M10,M11,M12,M13,M20,M21,M22,M23,M30,M31 00037000
                                                                          00038000
•M32 • M333
                                                                          00039000
SWITCH RETURN #=L10L20L30L40L50L60L73
INTEGER LOALF OALF OALF OBET OBET OBET OBET OBET OBET OBEST OF TALF OF TALF OF TALF OF TALF OBET OBET
.TBET.TBET1.TBET2.BETBEST.BESTM 3
                                                                          00041000
                                                                          00042000
ARRAY YOPY1[OBN];
PROCEDURE RECORDORDERS (Mo Xo XT o Yo YT) )
                                                                          00043000
VALUE MAXAXTAYAYTJ
                                                                          00044000
TNTEGER MOXOXTOYOYTJ
                                                                          00045000
                                                                          00046000
REGIN
                                                                          00047000
  KX *=KY *#1 +8×M3
                                                                          00048000
  KX. * # KX + 2 × X }
                                                                          00049000
  KY 8=KY +2×Y3
                                                                          00050000
                                                                          00051000
  IF XT <YT THEN
  BEGIN
                                                                          00052000
    Q[KY+1]:=Q[KY+1]-YT;
                                                                          00053000
    Q[KX] := Q[KX] + XT3
                                                                          00054000
                                                                          00055000
  ENDJ
                                                                          00056000
  IF YT <XT THEN
                                                                          00057000
  BEGIN
                                                                          00058000
    Q[KX+1] = Q[KX+1] = XTJ
                                                                          00059000
                                                                          00060000
    Q[KY ]:=Q[KY ]+YT;
                                                                          00061000
  END3
                                                                          00062000
                                                                          00063000
FND3
                                                                          00064000
PROCEDURE RECORDMETHODS(X,XT,Y,Y,YT);
                                                                          00065000
```

00066000	007000 007100 007100	007300 007300 007400	007500	007700	007900	008100	008200	008300	008800	008600	008700	008800	000600	009100	003500	008300	005600	009600	008500	006600	010000	010100	010200	000000000000000000000000000000000000000	000010

END;

PROCEDURE SELECTORDERS(M,X,Y);

INTEGER M,X,Y;

BEGIN

J:=J/@4;
FOR S :=0 STEP 1 UNTIL 3 DG

BEGIN
J:=(J+1)MOD 4;
K:=1 +8×M +2×J;

AT[S]:=Q[K]+Q[K+1];

BJ[S]:=J;

END

0[KY33 ]:=0[KY33 ]+YT; 0[KX41+1]:=0[KX41+1]=XT; 0[KY41 ]:=0[KY41 ]+YT;

Q[KX33+1]1 = Q[KX33+1] = XT

IF YT <XT THEN BEGIN

Q[KX33 ]:=Q[KX33 ]+XT; Q[KY41+1]:=Q[KY41+1]=YT;

Q[KX41 ] = Q[KX41 ] + XT ;

0[KY33+1]:=0[KY33+1]=YT

BEGIN

KX41 1=8 +KX33 +8×Y4 KY41 1=8 +KY33 +8×X4 IF XT <YT THEN

KX33 1833 +2XX3 KY33 1833 +2XY3

BEGIN

INTEGER XAXIAYAYTA

VALUE XAXTAYAYTS

```
X:=BJrol;
                                                                           00106000
      Y #= IF AT[1] AT[2] THEN IF AT[1] AT[3] THEN BU[1] ELSE BU[3] ELSE IF
                                                                           00107000
      ATT212ATT31THEN BJT21ELSE BJT313
                                                                           00108000
                                                                           00109000
    FND;
                                                                           00110000
    PROCEDURE SELECTMETHODS(X,Y);
                                                                           00111000
    INTEGER XOYS
                                                                           00112000
                                                                           00113000
    BEGIN
                                                                           00114000
      J:=Q[0]:=(Q[0]×4093 +3000001)MOD 16777216 ;
                                                                           00115000
      J 1=J/043
                                                                           00116000
      FOR S := 0 STEP 1 UNTIL 3 DO
                                                                           00117000
      BEGIN
                                                                           00118000
        J #=(J+1)MDD 43
                                                                           00119000
        K 1=33 +2×J;
                                                                           00120000
        AT[S]:=Q[K]+Q[K+1];
                                                                           00121000
        BJ[S] = J;
                                                                           00122000
                                                                           00123000
      END!
                                                                           00124000
      X:#BJ[0];
                                                                           00125000
      Y #= IF AT[1] AT[2] THEN IF AT[1] AT[3] THEN BJ[1] ELSE BJ[3] ELSE IF
                                                                           00126000
      ATT212ATT31THEN BJ121ELSE BJ131;
                                                                           00127000
                                                                           00128000
    END3
                                                                           00129000
    IF HEREBEFORE ≠"YES"THEN
                                                                           00130000
    BEGIN
                                                                           00131000
      LABEL L13
                                                                           00132000
      FILE IN TAPE831 2(2,90);
                                                                           00133000
      FORMAT FM ("SEND THIS HISTORY FILE AND THE PUNCHED CARDS TO L J GAO0134000
LLAHER VIA ", "CAMPUS MAIL"///X5, A5, I10, I10/(8110));
                                                                           00135000
      FORMAT FORM(/(5E20,11));
                                                                           00136000
     INTEGER J.K.S.
                                                                           00137000
      WHILE TRUE DO READ(A831HST,75,Q[*])[L18L1]8
                                                                           00138000
      L1:REWIND(A831HST);
                                                                           00139000
      COMMENT READ COEF . FILE !
                                                                           00140000
      FOR J == 0 STEP 1 UNTIL 3 DO FOR K 8=0 STEP 1 UNTIL 3 DO
                                                                           00141000
      BEGIN
                                                                           00142000
        IF J=2 AND K=0 THEN SPACE(TAPE831,1);
                                                                           00143000
        IF J=1 AND K=0 THEN SPACE(TAPE831,5);
                                                                           00144000
        READ(TAPE831,40,COEF[JoK,*]);
                                                                           00145000
```

\_

SWE4×BET+BET2+13;

00179000 00180000 00181000 00182000 00183000 00184000

00177000

00176000

00159000 00161000 00162000 00162000 00163000 00165000 00166000 00167000 00168000 00169000

00171000

00155000

00153000

00148000 00148000 00149000 00150000

00152000

00156000 00157000 00158000

```
1111
                                                                                                                    # 3 3 3 s
                   TBET2 :=TIME(2);
                                      WRITE(PUN +F2I1+BET+BET2);
                                                            SETYTANDY
                                                                             L3: TBET1 1=TIME(2)=TBET1;
                                                                                                GO TO SWE4×BET+BET1+13;
                                                                                                                                                          WRITE(PUN F2I1, BET, BET1);
                                                                                                                                                                               C = A + D D X ;
                                                                                                                                                                                                                                                           L2: TALF2 :=TIME(2)=TALF2;
                                                                                                                                                                                                                                                                               GO TO SW[4×ALF+ALF2+1];
                                                                                                                                                                                                                                                                                                   C##2;
                                                                                                                                                                                                                                                                                                                                        WRITE(PUN .F2I1, ALF, ALF2);
                                                                                                                                                                                                                                                                                                                                                              SETY! ANDY;
                                                                                                                                                                                                                                                                                                                                                                                LISTALF1 SHTIME(2)-TALF13
                                                                                                                                                                                                                                                                                                                                                                                                     GO TO SW[4×ALF+ALF1+1];
                                                                                                                                                                                                                                                                                                                                                                                                                        14
                                                                                                                                                                                                                                                                                                                                                                                                                                                            WRITE(PUN »F2I1» ALF» ALF1);
                                                                                                                                                                                                                                                                                                                                                                                                                                                                                  CIHA+DDX;
                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                          A : = C ;
                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                  SELECTORDERS(ALF, ALF1, ALF2);
                                                                                                                                      TBETT :=TIME(2);
                                                                                                                                                                                                18/([P]]A+[P]A)=: AAROA
                                                                                                                                                                                                                        A * # C ;
                                                                                                                                                                                                                                                                                                                       TALF? :=TIME(2);
                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                       FAABOA
                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                            UDX + = (XF = XI)/8;
                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                 SELECTORDERS (BET, BET1, BET2);
                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                        SELECTMETHODS (ALF, BET);
                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                           INTOVR := L39;
                                                                                                                                                                                                                                                                                                                                                                                                                                           TALF1 :=TIME(2);
                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                T 20
                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                       HEREBEFORE :="YES";
                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                          WRITE(PUN .FM.LST);
```

```
00186000
14: TRFT2 8=TIME(2)=TBET23
                                                                        00187000
AC3
                                                                        00188000
A 8 = C 3
                                                                        00189000
YOBYY :=(Y[J]+Y1[J])/2;
                                                                        00190000
C := A + DDX \times 2 
ALFBEST := IF TALF1 STALF2 THEN ALF1 ELSE ALF2;
                                                                        00191000
BETBEST := IF TBET1 STBET2 THEN BET1 ELSE BET2;
                                                                        00192000
                                                                        00193000
WRITE(PUN >F2I1 + ALF + ALFBEST);
                                                                        00194000
TALF :=TIME(2);
                                                                        00195000
L:#5;
                                                                        00196000
G'D TO SWE4×ALF+ALFBEST+1];
                                                                        00197000
L5:TALF :=TIME(2)=TALF 3
                                                                        00198000
SETY1ANDY3
                                                                        00199000
WRITE(PUN ,F2I1,BET,BETBEST);
                                                                        00200000
TBET :=TIME(2);
                                                                        00201000
1 1 = 63
                                                                        00202000
GO TO SWE4×BET+BETBEST+1];
                                                                        00203000
16:TBET :=TIME(2)=TBET >
                                                                        00204000
AC3
                                                                        00205000
A:=C;
                                                                        00206000
YOBYY :=(Y[J]+Y1[J])/2;
                                                                        00207000
CI=XEI
                                                                        00208000
FOR J :=1 STEP 1 UNTIL 40 DO Q[J]:=Q[J]:0.980;
RECORDORDERS(ALF, ALF1, TALF1, ALF2, TALF2);
                                                                        00209000
                                                                        00210000
RECORDORDERS(BET, BET1, TBET1, BET2, TBET2);
                                                                        00211000
RECORDMETHODS(ALF, TALF, BET, TBET);
                                                                         00212000
 0[-1]:=0[-1]+1;
                                                                         00213000
WRITE(A831HST,75,Q[*1))
WRITE(PUN .FM5I10.ALF.ALF1.ALF1.ALF2.ALF2.BET.BET1.BET1.BET. 00214000
                                                                         00215000
BET25TBET2, ALF, TALF, BET, TBET, Q[=1]);
                                                                         00216000
IF TALF STBET THEN
                                                                         00217000
 REGIN
                                                                         00218000
  BESTM :=ALF;
                                                                         00219000
  BESTO :=ALFBEST
                                                                         00220000
 END ELSE
                                                                         00221000
 REGIN
                                                                         00555000
   BESTM :=BET3
                                                                         00223000
   BESTO :=BETBEST
                                                                         00224000
 END3
                                                                         00225000
 L 1=73
```

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GO TO SW[4×BESTM +BESTU +1];	022600	
BEGIN	027700	
GU TO L29	052500	
00 * COMMENT *	023000	
ADAMS(NAAACaYaFaPa3aDXaEAagRaCOEF[Oa0a4]a4a4aCOEF[3a0a4]aSS ); Gn tn 1993	00231000	
O1:COMME	023300	
DAMSCNAAC	023400	
0 10 129;	023500	
02 s COMMENT s	003800	
DAMSCNA	023700	
0 TO L29;	023800	
0.3 * COMMENT?	023900	
A NU SWAU	054000	
0 10 1293	024100	
10 * COMMENTS	054500	
UTCHERCA	054300	
0 TO L29;	054400	
11 COMMENT'S	054200	
UTCHERCNA	024600	
0 TO L29	024700	
12 & COMMENT;	024800	
UTCHERON	054800	
0 TO L29	025000	
13 * COMMENT;	025100	
UTCHERON	025200	
0 TO L29;	025300	
20 COMMENT	025400	
DWELL CN.	025500	
0 TO L29	025600	
21 COMMENT;	025700	
OWELL CN, A,	025800	
0:T0 L29	025900	
22 COMMENT	026000	
OWELL(NAA)	026100	
0 TO L293	026200	
23 COMMENT!	026300	
OWELLCNAA	056400	
0 TO L29	026500	

M30 COMMENT;	00266000
SHANKS(NAAPCAYAFA4A4COEFE3AOA*JAPAEAAERADX);	00267000
GO TO L293	00268000
M31:COMMENT;	00269000
SHANKS(N,A,C,Y,F,5,5,COEF[3,1,*],P,EA,ER,DX);	00270000
GO TO L293	00271000
M32:COMMENT;	00272000
SHANKS(N,A,C,Y,F,6,6,COEF(3,2,*1,P,EA,ER,DX))	00273000
GO TO L291	00274000
M33:COMMENT)	00275000
'SHANKS(N,A,C,Y,F,7,7,COEF[3,3,*],P,EA,ER,DX);	00276000
L29:GO TO RETURN[L];	00277000
L39:WRITE(PUN,FMINTOVR);	00278000
	00279000
GO TO M30;	00280000
,	00281000
END;	00282000
L7:	00283000
END;	7 0 C 4 9 0 0 0

.

,我们就是不是我们的,我们就是一个一块,我们就是我们的,我们就是这个人的。""我们,我们就是我们的,我们就是一定。"

### IV. RESULTS AND CONCLUSIONS

### A. Applications

Three types of problems were used to exercise this integration procedure. The first type is the Arenstorf orbits of the restricted three body problem. The second is the system of linear differential equations associated with Fourier transforms. The third type is the system of linear equations obtained from a discretization of the partial differential equation for the vibrating string.

The first of these is characterized by the necessity of frequent step size change. The other two types are characterized by having a large number (20 to 100) of coupled equations.

### B. Results

The executive routine performed quite satisfactorily. Learning took place as was desired, the procedure adapting readily to the characteristics of a particular problem and accuracy.

The results of running with a variety of problems and accuracies are that no particular method seems to be exceptionally superior to any other. It did appear that for the accuracy range used (10<sup>-3</sup> to 10<sup>-9</sup>) certain orders of some methods were inappropriate. Also for a given method one particular order usually dominated, but which one dominated depended on the accuracy being asked and to some extent on the problem.

All methods performed well and, for different problems, different methods showed up more successfully. The Runge-Kutta-Shanks method was usually faster for problems where frequent step size changes were required, but the multi-step methods usually performed better when long runs of uniform step size

were appropriate. Of the multistep methods, that of Adams was usually the fastest.

The performance of the various orders of each method was as follows:

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For the Adams method, 6th order was best most often for these accuracies, with 5th order next fastest.

Of the Butcher formulas, the 5th order was most often the fastest. No clear cut case was established for second best, but it was evident that 9th order or higher was clearly too slow at these accuracies to be included among the possible orders.

For the Cowell method, 6th order was usually the best. 12th order and higher were too slow and should not be used at these accuracies.

Of the Shanks formulas, the 4th order was usually the fastest, with the 5th and 6th orders not too far behind.

## C. Conclusions

The results justify the conclusion that the present program would be suitable and effective as a general library program for integrating systems of differential equations. It was evident that no particular method or order is exceptionally superior to all the others. Depending on the accuracy and the problem, different methods and orders are best. The executive routine does a satisfactory job of finding a good method and order for each individual problem.

# D. Suggestions for Further Study

Several additional tasks and improvements to the present project can be envisioned.

The first additional task would be to convert the integration procedure to double precision (22 decimal places). This would allow an exploration

of a wider range of accuracies and order. Also at the higher accuracies more striking differences in the efficiencies of the various methods and orders are expected to occur. Experiments of the type carried out in single precision could then be done in double precision and the results extended over a wider range of accuracies and orders.

As a second additional task, a further investigation should be carried out into the correlation between order and accuracies. The present program does not try to anticipate the optimum order from the accuracy requirements. There should be a correlation between accuracy and optimum order. This could be built into the program either on an empirical basis or preferably as a learning function; that is, as a correlation to be learned by the program from the running experience.

A third suggestion for further work would be to make improvements in the learning mechanism. One such possibility just mentioned is to incorporate the learning of the correlation between order and accuracy. Also an investigation of the optimum rate of "forgetting" could be undertaken. The whole mechanism of learning should be investigated more thoroughly for the purpose of optimizing the learning process.

Other revisions in the program or extensions of this work would be to improve or refine the step size and error control, to do more experimenting with a wider variety of problems, and possibly to incorporate other integration methods into the program.

Respectfully submitted,

Í. E. Perlin Project Director

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